Annex II-6

Physicochemical Properties and Chemical Classes of Natural Complex Substances Tested in the LLNA

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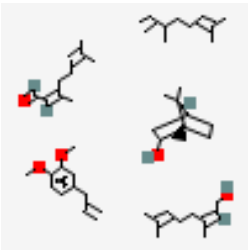
Substance Name	Synonyms	CASRN	Molecular Weight (g/mol)	Log Kow [1]	Physical Form	Chemical Class[2]	Structure[3]
Basil oil	Ocimum basilicum oil	8015-73-4	NA	NA	Liquid	Lipids	NA
Citronella oil	Cymbopogon nardus oil	8000-29-1	NA	3.53	Liquid	Lipids	NA
Clove Oil	Clove leaf oil Clove stem oil	8000-34-8	NA	NA	Liquid	Lipids	NA
Geranium oil	Geranium maculatum oil	8000-46-2	NA	NA	Liquid	NA	NA
Jasmine absolute	Gardenia jasminoides, ext.	92457-01-7	NA	NA	NA	NA	NA
Lemongrass oil	Citral terpenes; 1,2-dimethoxy-4-prop-2-enylbenzene	8007-02-1	777.21	NA	Liquid	NA	
Litsea cubeb oil	Litsea cubeba	68855-99-2	NA	NA	Liquid	NA	NA
Oakmoss	Oak moss extract, absolute	68917-10-2	NA	NA	NA	NA	NA
Palmarosa oil	Cymbopogon martini oil	8014-19-5	NA	NA	NA	NA	NA
Spearmint oil	Mentha spicata oil	8008-79-5	NA	NA	Liquid	NA	NA
Treemoss	Cedar moss extract	68648-41-9	NA	NA	NA	NA	NA
Ylang Ylang oil	Cananga oil	68606-83-7 8006-81-3	NA	NA	NA	NA	NA

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; g/mol = grams per mole; Kow = octanol-water partition coefficient; NA = not available.

[1]Kow represents the octanol-water partition coefficient (expressed on log scale) obtained from the website: http://www.syrres.com/esc/est_kowdemo.htm.

[2]Chemical classifications based on the Medical Subject Headings classification for chemicals and drugs, as developed by the National Library of Medicine at: http://www.nlm.nih.gov/mesh/meshhome.html

[3]Chemical structures, based on CASRN, were obtained from ChemID available at: http://chem.sis.nlm.gov/chemidplus/chemidheavy.jsp.