Patchouli alcohol

Other names:	(-)-Patchouli alcohol
	(-)-Patchoulol
	(1R,4S,4aS,6R,8aS)-4,8a,9,9-Tetramethyldecahydro-1,6-methanonaphthalen-1-ol
	1,6-Methanonaphthalen-1(2H)-ol, octahydro-4,8a,9,9-tetramethyl-, (1«alpha»,4«beta»,4a«alpha»,6«beta»,8a«alpha»)-
	1,6-Methanonaphthalen-1(2H)-ol, octahydro-4,8a,9,9-tetramethyl-, [1R-(1«alpha»,4«beta»,4a«alpha»,6«beta»,8a«alpha»)]-
	Patchoulanol
	Patchoulic alcohol
	[1R-(1«alpha»,4«beta»,4a«alpha»,6«beta»,8a«alpha»)]-octahydro-4,8a,9,9-tetramethyl-1
	patchoulol
Inchi:	InChI=1S/C15H26O/c1-10-5-8-15(16)13(2,3)11-6-7-14(15,4)12(10)9-11/h10-12,16H,5-9H
InchiKey:	GGHMUJBZYLPWFD-UIWQZIKGSA-N
Formula:	C15H26O
SMILES:	CC1CCC2(O)C(C)(C)C3CCC2(C)C1C3
Mol. weight [g/mol]:	222.37
CAS:	5986-55-0

Physical Properties

Property code	Value	Unit	Source
gf	57.05	kJ/mol	Joback Method
hf	-314.38	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	61.37	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.610		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1665.00		NIST Webbook

rinpol	1659.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1639.80		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1639.80		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1653.00		NIST Webbook
ripol	2188.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2186.00		NIST Webbook
tb	650.25	K	Joback Method
tc	863.66	K	Joback Method
tf	425.39	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.75	J/mol×K	650.25	Joback Method
cpg	615.74	J/mol×K	685.82	Joback Method
cpg	634.97	J/mol×K	721.39	Joback Method
cpg	653.76	J/mol×K	756.96	Joback Method
cpg	672.45	J/mol×K	792.52	Joback Method
cpg	691.37	J/mol×K	828.09	Joback Method
cpg	710.84	J/mol×K	863.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5986550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of the Sesquiterpene Alcohol Patchoulol in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je060358w
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume