«beta»-Vetispirene

Other names:	1,8a-dimethyl-7-propan-2-ylidene-1,2,6,8-tetrahydronaphthalene
	Naphthalene, 1,2,6,7,8,8a-hexahydro-1,8a-dimethyl-7-(1-methylethylidene)-, (1R,8aS)-
	4«beta»H,5«alpha»-Eremophila-1,7(11),9-triene
	«beta»-Vatirenene
	«beta»-Vetivenene
Inchi:	InChI=1S/C15H22/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h5,7,9,12H,6,8,10H2,1-4
InchiKey:	QSUQBXKPPUWLTH-DOMZBBRYSA-N
Formula:	C15H22
SMILES:	CC(C)=C1CC=C2C=CCC(C)C2(C)C1
Mol. weight [g/mol]:	202.34

Physical Properties

Property code	Value	Unit	Source
gf	230.23	kJ/mol	Joback Method
hf	-46.40	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	50.46	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.645		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	1574.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1554.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1488.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1868.00		NIST Webbook

ripol	1885.00		NIST Webbook
ripol	1852.00		NIST Webbook
ripol	1885.00		NIST Webbook
ripol	1864.00		NIST Webbook
tb	583.22	K	Joback Method
tc	812.62	K	Joback Method
tf	314.95	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.83	J/mol×K	583.22	Joback Method
cpg	502.10	J/mol×K	621.45	Joback Method
cpg	522.00	J/mol×K	659.69	Joback Method
cpg	540.71	J/mol×K	697.92	Joback Method
cpg	558.40	J/mol×K	736.15	Joback Method
cpg	575.26	J/mol×K	774.38	Joback Method
cpg	591.45	J/mol×K	812.62	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27840400&Units=SI

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