Vetivazulene

Inchi: InChI=1S/C15H18/c1-10(2)13-8-14-11(3)6-5-7-12(4)15(14)9-13/h5-10H,1-4H3
InchiKey: APVKGMMYGFJZHY-UHFFFAOYSA-N
Formula: C15H18
SMILES: Cc1cccc(C)c2cc(C(C)C)cc1-2
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	263.15	kJ/mol	Joback Method
hf	34.98	kJ/mol	Joback Method
hfus	20.98	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.532		Crippen Method
mcvol	178.990	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1787.00		NIST Webbook
rinpol	1787.00		NIST Webbook
tb	602.76	K	Joback Method
tc	827.42	K	Joback Method
tf	340.49	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.16	J/mol×K	602.76	Joback Method
cpg	514.60	J/mol×K	789.98	Joback Method
cpg	501.39	J/mol×K	752.54	Joback Method
cpg	487.31	J/mol×K	715.09	Joback Method
cpg	472.29	J/mol×K	677.65	Joback Method
cpg	456.26	J/mol×K	640.20	Joback Method
cpg	526.98	J/mol×K	827.42	Joback Method
dvisc	0.0002427	Pa×s	602.76	Joback Method

dvisc	0.0002889	Pa×s	559.05	Joback Method
dvisc	0.0003542	Pa×s	515.34	Joback Method
dvisc	0.0004510	Pa×s	471.62	Joback Method
dvisc	0.0006032	Pa×s	427.91	Joback Method
dvisc	0.0008620	Pa×s	384.20	Joback Method
dvisc	0.0013500	Pa×s	340.49	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=R281686&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume