

«beta»-vetivene

Inchi:	InChI=1S/C15H24/c1-9(2)13-7-14-10(3)11-4-5-12(6-11)15(14)8-13/h9,11-15H,3-8H2,1-2
InchiKey:	DFUVGLKCF AASAU-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C1C2CCC(C2)C2CC(C(C)C)CC12
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	268.69	kJ/mol	Joback Method
hf	-108.57	kJ/mol	Joback Method
hfus	22.27	kJ/mol	Joback Method
hvap	48.22	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1546.00		NIST Webbook
tb	560.74	K	Joback Method
tc	772.34	K	Joback Method
tf	295.79	K	Joback Method
vc	0.707	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.34	J/mol×K	560.74	Joback Method
cpg	609.83	J/mol×K	737.08	Joback Method
cpg	591.32	J/mol×K	701.81	Joback Method
cpg	571.61	J/mol×K	666.54	Joback Method
cpg	550.59	J/mol×K	631.27	Joback Method

cpg	528.20	J/molxK	596.01	Joback Method
cpg	627.20	J/molxK	772.34	Joback Method
dvisc	0.0014896	Paxs	560.74	Joback Method
dvisc	0.0014878	Paxs	516.58	Joback Method
dvisc	0.0014857	Paxs	472.42	Joback Method
dvisc	0.0014831	Paxs	428.26	Joback Method
dvisc	0.0014799	Paxs	384.11	Joback Method
dvisc	0.0014760	Paxs	339.95	Joback Method
dvisc	0.0014709	Paxs	295.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R238192&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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