

Sesquisabinene

Inchi:	InChI=1S/C15H24/c1-11(2)6-5-7-13(4)15-9-8-12(3)14(15)10-15/h6,13-14H,3,5,7-10H2,1
InchiKey:	DYUSFBWNOCHOFFP-JVIGXAJISA-N
Formula:	C15H24
SMILES:	C=C1CCC2(C(C)CCC=C(C)C)CC12
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	313.74	kJ/mol	Joback Method
hf	-5.70	kJ/mol	Joback Method
hfus	18.79	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1476.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1461.00		NIST Webbook
tb	559.08	K	Joback Method
tc	762.67	K	Joback Method
tf	298.23	K	Joback Method
vc	0.747	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.68	J/molxK	559.08	Joback Method
cpg	513.41	J/molxK	593.01	Joback Method

cpg	531.88	J/mol×K	626.94	Joback Method
cpg	549.25	J/mol×K	660.88	Joback Method
cpg	565.68	J/mol×K	694.81	Joback Method
cpg	581.34	J/mol×K	728.74	Joback Method
cpg	596.38	J/mol×K	762.67	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R610534&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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