Sesquisabinene A

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: DYUSFBWNOCHOFP-SHARSMKWSA-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	1446.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook
ripol	1629.00		NIST Webbook
tb	559.08	K	Joback Method
tc	762.67	K	Joback Method
tf	298.23	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R431297&Units=SI
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

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

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