Sesquisabinene B

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-RRFJBIMHSA-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
hfus	18.79	kJ/mol	Joback Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1446.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1446.00		NIST Webbook
tb	523.93	K	Cheméo Relay (1.0)

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R620912&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature