

«alpha»-Bisabolone oxide A

Inchi:	InChI=1S/C15H26O2/c1-11-5-7-12(8-6-11)15(4)10-9-13(16)14(2,3)17-15/h5,12-13,16H,6
InchiKey:	WJHRAVIQWFQMKF-RGPPAHDHSA-N
Formula:	C15H26O2
SMILES:	CC1=CCC(C2(C)CCC(O)C(C)(C)O2)CC1
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-104.69	kJ/mol	Joback Method
hf	-492.41	kJ/mol	Joback Method
hfus	20.72	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.441		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	1633.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1686.00		NIST Webbook
ripol	2132.00		NIST Webbook
ripol	2104.00		NIST Webbook
tb	696.11	K	Joback Method
tc	915.11	K	Joback Method
tf	413.56	K	Joback Method
vc	0.761	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	634.07	J/mol×K	696.11	Joback Method
cpg	654.68	J/mol×K	732.61	Joback Method
cpg	674.52	J/mol×K	769.11	Joback Method
cpg	693.78	J/mol×K	805.61	Joback Method
cpg	712.67	J/mol×K	842.11	Joback Method
cpg	731.40	J/mol×K	878.61	Joback Method
cpg	750.18	J/mol×K	915.11	Joback Method

Sources

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=R600547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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