

«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-RLSDIYDTSA-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	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1669.00		NIST Webbook
tb	696.11	K	Joback Method
tc	915.11	K	Joback Method
tf	413.56	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

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=R199790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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