«alpha»-Bisabolenal

Inchi: InChI=1S/C15H22O/c1-12(2)5-4-6-13(3)15-9-7-14(11-16)8-10-15/h5-7,11,15H,4,8-10H2,
InchiKey: QKYFEBFAJXZXEK-MLPAPPSSSA-N
Formula: C15H22O
SMILES: CC(C)=CCC=C(C)C1CC=C(C=O)CC1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	164.02	kJ/mol	Joback Method
hf	-123.02	kJ/mol	Joback Method
hfus	27.35	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook
tb	623.03	K	Joback Method
tc	837.21	K	Joback Method
tf	283.39	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.58	J/mol×K	623.03	Joback Method
cpg	540.58	J/mol×K	658.73	Joback Method
cpg	558.40	J/mol×K	694.42	Joback Method
cpg	575.13	J/mol×K	730.12	Joback Method
cpg	590.82	J/mol×K	765.82	Joback Method
cpg	605.54	J/mol×K	801.51	Joback Method
cpg	619.37	J/mol×K	837.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R324486&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume