Bisabolone

Inchi: InChI=1S/C15H26O/c1-11(2)15(16)10-7-13(4)14-8-5-12(3)6-9-14/h5,11,13-14H,6-10H2,1
InchiKey: FFZCGQYOMOOQNB-UHFFFAOYSA-N
Formula: C15H26O
SMILES: CC1=CCC(C(C)CCC(=O)C(C)C)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	-13.60	kJ/mol	Joback Method
hf	-375.44	kJ/mol	Joback Method
hfus	21.83	kJ/mol	Joback Method
hvap	56.34	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.374		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1750.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
ripol	2036.00		NIST Webbook
ripol	2036.00		NIST Webbook
tb	619.28	K	Joback Method
tc	822.53	K	Joback Method
tf	299.40	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.79	J/mol×K	619.28	Joback Method
cpg	654.89	J/mol×K	788.65	Joback Method
cpg	638.80	J/mol×K	754.78	Joback Method
cpg	621.69	J/mol×K	720.90	Joback Method

cpg	603.50	J/mol×K	687.03	Joback Method
cpg	584.21	J/mol×K	653.15	Joback Method
cpg	669.97	J/mol×K	822.53	Joback Method
dvisc	0.0001640	Pa×s	619.28	Joback Method
dvisc	0.0002230	Pa×s	565.97	Joback Method
dvisc	0.0003234	Pa×s	512.65	Joback Method
dvisc	0.0005111	Pa×s	459.34	Joback Method
dvisc	0.0009111	Pa×s	406.03	Joback Method
dvisc	0.0019340	Pa×s	352.71	Joback Method
dvisc	0.0053674	Pa×s	299.40	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=R239655&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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