Bulnesyl acetate

Inchi: InChI=1S/C17H28O2/c1-11-6-8-14(17(4,5)19-13(3)18)10-16-12(2)7-9-15(11)16/h12,14,1
InchiKey: JBVWTNIISBARDE-SCYXSXAHSA-N
Formula: C17H28O2
SMILES: CC(=O)OC(C)(C)C1CCC(C)=C2CCC(C)C2C1
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	-62.73	kJ/mol	Joback Method
hf	-512.30	kJ/mol	Joback Method
hfus	24.54	kJ/mol	Joback Method
hvap	63.12	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.491		Crippen Method
mcvol	231.810	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2156.00		NIST Webbook
tb	696.43	K	Joback Method
tc	914.62	K	Joback Method
tf	399.29	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.93	J/mol×K	696.43	Joback Method
cpg	719.94	J/mol×K	732.80	Joback Method
cpg	740.52	J/mol×K	769.16	Joback Method
cpg	759.70	J/mol×K	805.53	Joback Method
cpg	777.56	J/mol×K	841.89	Joback Method
cpg	794.15	J/mol×K	878.26	Joback Method

cpg	809.53	J/mol×K	914.62	Joback Method
dvisc	0.0018116	Pa×s	399.29	Joback Method
dvisc	0.0010728	Pa×s	448.81	Joback Method
dvisc	0.0007051	Pa×s	498.34	Joback Method
dvisc	0.0004999	Pa×s	547.86	Joback Method
dvisc	0.0003752	Pa×s	597.38	Joback Method
dvisc	0.0002943	Pa×s	646.91	Joback Method
dvisc	0.0002389	Pa×s	696.43	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=R344386&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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