Bornyl hexanoate

Inchi: InChI=1S/C16H28O2/c1-5-6-7-8-14(17)18-13-11-12-9-10-16(13,4)15(12,2)3/h12-13H,5-1
InchiKey: FVTTUTDGUCSLMA-UYJPIKCFSA-N
Formula: C16H28O2
SMILES: CCCCCC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]: 252.39

Physical Properties

Property code	Value	Unit	Source
gf	-67.08	kJ/mol	Joback Method
hf	-489.13	kJ/mol	Joback Method
hfus	23.70	kJ/mol	Joback Method
hvap	57.44	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.325		Crippen Method
mcvol	222.020	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	650.66	K	Joback Method
tc	853.25	K	Joback Method
tf	413.92	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.70	J/mol×K	650.66	Joback Method
cpg	667.95	J/mol×K	684.43	Joback Method
cpg	687.34	J/mol×K	718.19	Joback Method
cpg	706.08	J/mol×K	751.96	Joback Method
cpg	724.33	J/mol×K	785.72	Joback Method
cpg	742.31	J/mol×K	819.49	Joback Method
cpg	760.20	J/mol×K	853.25	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=R224712&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