

Longiborneol acetate

Inchi:	InChI=1S/C17H28O2/c1-11(18)19-14-13-12-7-10-17(14,5)16(12,4)9-6-8-15(13,2)3/h12-1
InchiKey:	NVBYJWWRRWURRN-FECYRMIVSA-N
Formula:	C17H28O2
SMILES:	CC(=O)OC1C2C3CCC1(C)C3(C)CCCC2(C)C
Mol. weight [g/mol]:	264.40

Physical Properties

Property code	Value	Unit	Source
hfus	17.10	kJ/mol	Joback Method
logp	4.181		Crippen Method
mcvol	225.250	ml/mol	McGowan Method
rinpol	1687.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.49	J/mol×K	680.12	Joback Method
cpg	713.37	J/mol×K	717.86	Joback Method
cpg	735.56	J/mol×K	755.59	Joback Method
cpg	757.45	J/mol×K	793.33	Joback Method
cpg	779.41	J/mol×K	831.06	Joback Method
cpg	801.82	J/mol×K	868.80	Joback Method
cpg	825.06	J/mol×K	906.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R609262&Units=SI

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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