

Sobrerol 8-acetate

Inchi:	InChI=1S/C12H20O3/c1-8-5-6-10(7-11(8)14)12(3,4)15-9(2)13/h5,10-11,14H,6-7H2,1-4H
InchiKey:	ISKWEZUCHJMRLH-UHFFFAOYSA-N
Formula:	C12H20O3
SMILES:	CC(=O)OC(C)(C)C1CC=C(C)C(O)C1
Mol. weight [g/mol]:	212.29
CAS:	93133-02-9

Physical Properties

Property code	Value	Unit	Source
gf	-280.67	kJ/mol	Joback Method
hf	-616.50	kJ/mol	Joback Method
hfus	20.04	kJ/mol	Joback Method
hvap	67.92	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.045		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1528.80		NIST Webbook
tb	658.22	K	Joback Method
tc	858.39	K	Joback Method
tf	376.82	K	Joback Method
vc	0.657	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.00	J/molxK	658.22	Joback Method
cpg	519.66	J/molxK	691.58	Joback Method
cpg	534.39	J/molxK	724.94	Joback Method
cpg	548.21	J/molxK	758.30	Joback Method
cpg	561.14	J/molxK	791.67	Joback Method
cpg	573.22	J/molxK	825.03	Joback Method
cpg	584.46	J/molxK	858.39	Joback Method
dvisc	0.0030088	Paxs	376.82	Joback Method

dvisc	0.0010767	Paxs	423.72	Joback Method
dvisc	0.0004729	Paxs	470.62	Joback Method
dvisc	0.0002411	Paxs	517.52	Joback Method
dvisc	0.0001375	Paxs	564.42	Joback Method
dvisc	0.0000855	Paxs	611.32	Joback Method
dvisc	0.0000568	Paxs	658.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93133029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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