

Juniperol acetate

Inchi:

lnchl=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-JULPFRMLSA-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
gf	-23.21	kJ/mol	Joback Method
hf	-448.23	kJ/mol	Joback Method
hfus	17.10	kJ/mol	Joback Method
hvap	58.30	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.181		Crippen Method
mcvol	225.250	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1679.00		NIST Webbook
tb	680.12	K	Joback Method
tc	906.53	K	Joback Method
tf	459.27	K	Joback Method
vc	0.858	m3/kmol	Joback Method

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:	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=R440503&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
hvac:	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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