Ledol, acetate

Inchi: InChI=1S/C17H28O2/c1-10-6-7-12-14(10)15-13(16(15,3)4)8-9-17(12,5)19-11(2)18/h10,1
InchiKey: RBKZSYFCQJXCHB-CJZKUJKOSA-N
Formula: C17H28O2
SMILES: CC(=O)OC1(C)CCC2C(C3C(C)CCC31)C2(C)C
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	-25.43	kJ/mol	Joback Method
hf	-483.81	kJ/mol	Joback Method
hfus	24.47	kJ/mol	Joback Method
hvap	59.14	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	4.037		Crippen Method
mcvol	225.250	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	1714.00		NIST Webbook
tb	675.21	K	Joback Method
tc	893.84	K	Joback Method
tf	431.13	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.04	J/mol×K	675.21	Joback Method
cpg	719.23	J/mol×K	711.65	Joback Method
cpg	741.42	J/mol×K	748.09	Joback Method
cpg	762.89	J/mol×K	784.53	Joback Method
cpg	783.85	J/mol×K	820.97	Joback Method
cpg	804.57	J/mol×K	857.40	Joback Method
cpg	825.29	J/mol×K	893.84	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=R410730&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