Oplopanoyl acetate

Other names: Oplopanonyl acetate
Inchi: InChI=1S/C17H28O3/c1-10(2)13-8-9-17(5,20-12(4)19)15-7-6-14(11(3)18)16(13)15/h10,1
InchiKey: DMVJXSFUJUHRRF-UHFFFAOYSA-N
Formula: C17H28O3
SMILES: CC(=O)OC1(C)CCC(C(C)C)C2C(C(C)=O)CCC21
Mol. weight [g/mol]: 280.40
CAS: 132032-86-1

Physical Properties

Property code	Value	Unit	Source
gf	-216.44	kJ/mol	Joback Method
hf	-675.53	kJ/mol	Joback Method
hfus	27.53	kJ/mol	Joback Method
hvap	67.21	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.606		Crippen Method
mcvol	237.680	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	1890.10		NIST Webbook
rinpol	1881.00		NIST Webbook
rinpol	1890.10		NIST Webbook
rinpol	1881.00		NIST Webbook
tb	730.60	K	Joback Method
tc	945.41	K	Joback Method
tf	424.94	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.40	J/mol×K	730.60	Joback Method
cpg	765.87	J/mol×K	766.40	Joback Method
cpg	786.29	J/mol×K	802.20	Joback Method
cpg	805.78	J/mol×K	838.00	Joback Method

cpg	824.45	J/mol×K	873.80	Joback Method
cpg	842.43	J/mol×K	909.60	Joback Method
cpg	859.84	J/mol×K	945.41	Joback Method

Sources

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=C132032861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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