10-Acetoxyneryl isobutyrate

Inchi: InChI=1S/C17H28O4/c1-13(2)7-6-8-16(12-21-15(5)18)9-10-20-17(19)11-14(3)4/h7,9,14H
InchiKey: WYNIMBPRCCVMCX-CXUHLZMHSA-N
Formula: C17H28O4
SMILES: CC(=O)OCC(=CCOC(=O)CC(C)C)CCC=C(C)C
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-234.68	kJ/mol	Joback Method
hf	-674.23	kJ/mol	Joback Method
hfus	39.62	kJ/mol	Joback Method
hvap	71.44	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.812		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1783.00		NIST Webbook
ripol	2347.00		NIST Webbook
ripol	2347.00		NIST Webbook
tb	748.58	K	Joback Method
tc	939.77	K	Joback Method
tf	372.59	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.12	J/mol×K	748.58	Joback Method
cpg	759.56	J/mol×K	780.44	Joback Method
cpg	775.10	J/mol×K	812.31	Joback Method
cpg	789.79	J/mol×K	844.17	Joback Method
cpg	803.65	J/mol×K	876.04	Joback Method
cpg	816.70	J/mol×K	907.90	Joback Method

cpg	829.00	J/mol×K	939.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R518171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume