8-Isobutyryloxy isobornyl isobutyrate

Inchi: InChI=1S/C18H30O4/c1-11(2)15(19)21-10-18(6)13-7-8-17(18,5)14(9-13)22-16(20)12(3)4
InchiKey: TYRVJKXVESQUNB-FSNFEAPFSA-N
Formula: C18H30O4
SMILES: CC(C)C(=O)OCC1(C)C2CCC1(C)C(OC(=O)C(C)C)C2
Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	-289.04	kJ/mol	Joback Method
hf	-785.77	kJ/mol	Joback Method
hfus	24.62	kJ/mol	Joback Method
hvap	70.28	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.580		Crippen Method
mcvol	257.640	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	1866.00		NIST Webbook
rinpol	1869.00		NIST Webbook
tb	771.83	K	Joback Method
tc	981.22	K	Joback Method
tf	478.62	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.71	J/mol×K	771.83	Joback Method
cpg	840.36	J/mol×K	806.73	Joback Method
cpg	860.64	J/mol×K	841.63	Joback Method
cpg	880.73	J/mol×K	876.53	Joback Method
cpg	900.84	J/mol×K	911.43	Joback Method
cpg	921.17	J/mol×K	946.32	Joback Method
cpg	941.91	J/mol×K	981.22	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R288003&Units=SI

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