Isobornyl caprate

Inchi: InChI=1S/C20H36O2/c1-5-6-7-8-9-10-11-12-18(21)22-17-15-16-13-14-20(17,4)19(16,2)3
InchiKey: JZDLFGOESWNMDS-UHFFFAOYSA-N
Formula: C20H36O2
SMILES: CCCCCCCCCC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]: 308.50

Physical Properties

Property code	Value	Unit	Source
gf	-33.40	kJ/mol	Joback Method
hf	-571.69	kJ/mol	Joback Method
hfus	34.06	kJ/mol	Joback Method
hvap	66.35	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.885		Crippen Method
mcvol	278.380	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	2087.60		NIST Webbook
rinpol	2087.60		NIST Webbook
tb	742.18	K	Joback Method
tc	937.02	K	Joback Method
tf	459.00	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.70	J/mol×K	742.18	Joback Method
cpg	900.67	J/mol×K	774.65	Joback Method
cpg	922.10	J/mol×K	807.13	Joback Method
cpg	943.16	J/mol×K	839.60	Joback Method
cpg	964.03	J/mol×K	872.07	Joback Method
cpg	984.90	J/mol×K	904.55	Joback Method
cpg	1005.94	J/mol×K	937.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414149&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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