Isobornyl isovalerate

Inchi: InChI=1S/C15H26O2/c1-10(2)8-13(16)17-12-9-11-6-7-15(12,5)14(11,3)4/h10-12H,6-9H2
InchiKey: MPYYVGIJHREDBO-AVERBVTBSA-N
Formula: C15H26O2
SMILES: CC(C)CC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-77.94	kJ/mol	Joback Method
hf	-473.77	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	54.83	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.790		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1516.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1530.00		NIST Webbook
tb	627.34	K	Joback Method
tc	836.82	K	Joback Method
tf	387.65	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.55	J/mol×K	627.34	Joback Method
cpg	613.85	J/mol×K	662.25	Joback Method
cpg	633.16	J/mol×K	697.17	Joback Method
cpg	651.71	J/mol×K	732.08	Joback Method
cpg	669.68	J/mol×K	766.99	Joback Method

cpg	687.30	J/mol×K	801.90	Joback Method
cpg	704.76	J/mol×K	836.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U109299&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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