«beta»-Alanine, N-isobutyryl-, undecyl ester

Inchi: InChI=1S/C18H35NO3/c1-4-5-6-7-8-9-10-11-12-15-22-17(20)13-14-19-18(21)16(2)3/h16
InchiKey: QODWLHVQSNRPTM-UHFFFAOYSA-N
Formula: C18H35NO3
SMILES: CCCCCCCCCCCOC(=O)CCNC(=O)C(C)C
Mol. weight [g/mol]: 313.48

Physical Properties

Property code	Value	Unit	Source
gf	-175.21	kJ/mol	Joback Method
hf	-724.04	kJ/mol	Joback Method
hfus	48.34	kJ/mol	Joback Method
hvap	77.61	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.223		Crippen Method
mcvol	283.470	ml/mol	McGowan Method
pc	1261.06	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	791.13	K	Joback Method
tc	975.23	K	Joback Method
tf	452.37	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.26	J/mol×K	791.13	Joback Method
cpg	899.59	J/mol×K	821.81	Joback Method
cpg	915.96	J/mol×K	852.50	Joback Method
cpg	931.39	J/mol×K	883.18	Joback Method
cpg	945.90	J/mol×K	913.86	Joback Method
cpg	959.51	J/mol×K	944.54	Joback Method
cpg	972.26	J/mol×K	975.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321669&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