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

Inchi: InChI=1S/C13H25NO3/c1-4-5-6-7-10-17-12(15)8-9-14-13(16)11(2)3/h11H,4-10H2,1-3H3
InchiKey: RNHGEORTQJOUKK-UHFFFAOYSA-N
Formula: C13H25NO3
SMILES: CCCCCCOC(=O)CCNC(=O)C(C)C
Mol. weight [g/mol]: 243.34

Physical Properties

Property code	Value	Unit	Source
gf	-217.31	kJ/mol	Joback Method
hf	-620.84	kJ/mol	Joback Method
hfus	35.39	kJ/mol	Joback Method
hvap	66.48	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.272		Crippen Method
mcvol	213.020	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1808.00		NIST Webbook
rinpol	1808.00		NIST Webbook
tb	676.73	K	Joback Method
tc	858.60	K	Joback Method
tf	396.02	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.92	J/mol×K	676.73	Joback Method
cpg	613.24	J/mol×K	707.04	Joback Method
cpg	627.80	J/mol×K	737.35	Joback Method
cpg	641.61	J/mol×K	767.67	Joback Method
cpg	654.68	J/mol×K	797.98	Joback Method
cpg	667.03	J/mol×K	828.29	Joback Method
cpg	678.67	J/mol×K	858.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321664&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