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

Inchi: InChI=1S/C12H23NO3/c1-4-5-6-9-16-11(14)7-8-13-12(15)10(2)3/h10H,4-9H2,1-3H3,(H,1
InchiKey: YEPNMEFJNCDNMZ-UHFFFAOYSA-N
Formula: C12H23NO3
SMILES: CCCCCOC(=O)CCNC(=O)C(C)C
Mol. weight [g/mol]: 229.32

Physical Properties

Property code	Value	Unit	Source
gf	-225.73	kJ/mol	Joback Method
hf	-600.20	kJ/mol	Joback Method
hfus	32.80	kJ/mol	Joback Method
hvap	64.26	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.882		Crippen Method
mcvol	198.930	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1705.00		NIST Webbook
tb	653.85	K	Joback Method
tc	836.74	K	Joback Method
tf	384.75	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.56	J/mol×K	653.85	Joback Method
cpg	559.39	J/mol×K	684.33	Joback Method
cpg	573.50	J/mol×K	714.81	Joback Method
cpg	586.89	J/mol×K	745.30	Joback Method
cpg	599.58	J/mol×K	775.78	Joback Method
cpg	611.57	J/mol×K	806.26	Joback Method
cpg	622.88	J/mol×K	836.74	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=U321663&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