

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C14H27NO3/c1-4-5-6-7-8-11-18-13(16)9-10-15-14(17)12(2)3/h12H,4-11H2,1-3H

ZTKFUAHTBBMCEA-UHFFFAOYSA-N

C14H27NO3

CCCCCCCOC(=O)CCNC(=O)C(C)C

257.37

Physical Properties

Property code	Value	Unit	Source
gf	-208.89	kJ/mol	Joback Method
hf	-641.48	kJ/mol	Joback Method
hfus	37.98	kJ/mol	Joback Method
hvap	68.71	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.662		Crippen Method
mcvol	227.110	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	699.61	K	Joback Method
tc	880.88	K	Joback Method
tf	407.29	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.56	J/mol×K	699.61	Joback Method
cpg	668.33	J/mol×K	729.82	Joback Method
cpg	683.30	J/mol×K	760.03	Joback Method
cpg	697.48	J/mol×K	790.25	Joback Method
cpg	710.90	J/mol×K	820.46	Joback Method
cpg	723.56	J/mol×K	850.67	Joback Method
cpg	735.48	J/mol×K	880.88	Joback Method

Sources

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=U321665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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