.BETA.-alanine, n-isobutyryl-, heptyl ester

Inchi: InChI=1S/C14H27NO3/c1-4-5-6-7-8-11-18-13(16)9-10-15-14(17)12(2)3/h12H,4-11H2,1-3
InchiKey: ZTKFUAHTBBMCEA-UHFFFAOYSA-N
Formula: C14H27NO3
SMILES: CCCCCCCOC(=O)CCNC(=O)C(C)C
Mol. weight [g/mol]: 257.37

Physical Properties

Property code	Value	Unit	Source
hf	-787.03	kJ/mol	Cheméo Relay (1.0)
hfus	37.98	kJ/mol	Joback Method
hvap	82.71	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.03		Cheméo Relay (1.0)
logp	2.662		Crippen Method
mcvol	227.110	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1908.00		NIST Webbook
tb	563.79	K	Cheméo Relay (1.0)
tc	755.66	K	Cheméo Relay (1.0)
tf	291.99	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321665&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
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

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