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

Inchi: InChI=1S/C15H29NO3/c1-4-5-6-7-8-9-12-19-14(17)10-11-16-15(18)13(2)3/h13H,4-12H2
InchiKey: FUOMJHAVSXSVHV-UHFFFAOYSA-N
Formula: C15H29NO3
SMILES: CCCCCCCCOC(=O)CCNC(=O)C(C)C
Mol. weight [g/mol]: 271.40

Physical Properties

Property code	Value	Unit	Source
hf	-807.79	kJ/mol	Cheméo Relay (1.0)
hfus	40.57	kJ/mol	Joback Method
hvap	86.34	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.43		Cheméo Relay (1.0)
logp	3.052		Crippen Method
mcvol	241.200	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook
tb	572.19	K	Cheméo Relay (1.0)
tc	766.30	K	Cheméo Relay (1.0)
tf	296.86	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.39	J/mol×K	722.49	Joback Method
cpg	724.58	J/mol×K	752.68	Joback Method
cpg	739.93	J/mol×K	782.87	Joback Method
cpg	754.45	J/mol×K	813.06	Joback Method
cpg	768.17	J/mol×K	843.25	Joback Method
cpg	781.11	J/mol×K	873.44	Joback Method
cpg	793.27	J/mol×K	903.63	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321666&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

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