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

Inchi: InChI=1S/C19H37NO3/c1-4-5-6-7-8-9-10-11-12-13-16-23-18(21)14-15-20-19(22)17(2)3/l
InchiKey: FRHKQFCECXOUNC-UHFFFAOYSA-N
Formula: C19H37NO3
SMILES: CCCCCCCCCCCCOC(=O)CCN=C(O)C(C)C
Mol. weight [g/mol]: 327.50

Physical Properties

Property code	Value	Unit	Source
hf	-765.37	kJ/mol	Joback Method
hvap	86.73	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.453		Crippen Method
mcvol	297.560	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	878.71	K	Joback Method
tc	1075.98	K	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=U321670&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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