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

Inchi: InChI=1S/C10H19NO3/c1-4-7-14-9(12)5-6-11-10(13)8(2)3/h8H,4-7H2,1-3H3,(H,11,13)
InchiKey: YRGUXIFUHXGBAZ-UHFFFAOYSA-N
Formula: C10H19NO3
SMILES: CCCOC(=O)CCN=C(O)C(C)C
Mol. weight [g/mol]: 201.26

Physical Properties

Property code	Value	Unit	Source
hf	-579.61	kJ/mol	Joback Method
hvap	66.70	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.942		Crippen Method
mcvol	170.750	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1508.00		NIST Webbook
rinpol	1508.00		NIST Webbook
tb	672.79	K	Joback Method
tc	858.54	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=U321662&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