«beta»-Alanine, N-acryloyl-, isobutyl ester

Inchi: InChI=1S/C10H17NO3/c1-4-9(12)11-6-5-10(13)14-7-8(2)3/h4,8H,1,5-7H2,2-3H3,(H,11,1
InchiKey: AJCDVZHADBTWCQ-UHFFFAOYSA-N
Formula: C10H17NO3
SMILES: C=CC(O)=NCCC(=O)OCC(C)C
Mol. weight [g/mol]: 199.25

Physical Properties

Property code	Value	Unit	Source
hf	-454.18	kJ/mol	Joback Method
hvap	66.03	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.718		Crippen Method
mcvol	166.450	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1541.00		NIST Webbook
rinpol	1541.00		NIST Webbook
tb	669.47	K	Joback Method
tc	857.90	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U321676&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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