

DL-Alanine, N-methyl-N-hexyloxycarbonyl-, isobutyl ester

Inchi:	InChI=1S/C15H29NO4/c1-6-7-8-9-10-19-15(18)16(5)13(4)14(17)20-11-12(2)3/h12-13H,6
InchiKey:	GEJZLUVDLBSGQP-UHFFFAOYSA-N
Formula:	C15H29NO4
SMILES:	CCCCCOC(=O)N(C)C(C)C(=O)OCC(C)C
Mol. weight [g/mol]:	287.40

Physical Properties

Property code	Value	Unit	Source
gf	-286.52	kJ/mol	Joback Method
hf	-785.56	kJ/mol	Joback Method
hfus	36.15	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.223		Crippen Method
mcvol	247.070	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	1813.00		NIST Webbook
rinpol	1813.00		NIST Webbook
tb	706.74	K	Joback Method
tc	886.30	K	Joback Method
tf	405.60	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.05	J/molxK	706.74	Joback Method
cpg	735.81	J/molxK	736.67	Joback Method
cpg	751.71	J/molxK	766.59	Joback Method
cpg	766.75	J/molxK	796.52	Joback Method
cpg	780.95	J/molxK	826.45	Joback Method
cpg	794.33	J/molxK	856.38	Joback Method
cpg	806.88	J/molxK	886.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U392632&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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