

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

Inchi:	InChI=1S/C15H29NO4/c1-5-7-9-10-12-20-15(18)16(4)13(3)14(17)19-11-8-6-2/h13H,5-12
InchiKey:	GHXJKEKRNQWEQU-UHFFFAOYSA-N
Formula:	C15H29NO4
SMILES:	CCCCCOC(=O)N(C)C(C)C(=O)OCCCC
Mol. weight [g/mol]:	287.40

Physical Properties

Property code	Value	Unit	Source
gf	-284.08	kJ/mol	Joback Method
hf	-780.28	kJ/mol	Joback Method
hfus	39.68	kJ/mol	Joback Method
hvap	68.95	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.367		Crippen Method
mcvol	247.070	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	1855.00		NIST Webbook
rinpol	1855.00		NIST Webbook
tb	707.18	K	Joback Method
tc	884.66	K	Joback Method
tf	420.60	K	Joback Method
vc	0.935	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.57	J/mol×K	707.18	Joback Method
cpg	735.12	J/mol×K	736.76	Joback Method
cpg	750.83	J/mol×K	766.34	Joback Method
cpg	765.71	J/mol×K	795.92	Joback Method
cpg	779.77	J/mol×K	825.50	Joback Method
cpg	793.04	J/mol×K	855.08	Joback Method
cpg	805.51	J/mol×K	884.66	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=U392633&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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