

Glycine, N-methyl-N-butoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C14H27NO4/c1-5-6-9-19-14(17)15(4)11-13(16)18-10-7-8-12(2)3/h12H,5-11H2
InchiKey: IKXXFOCSUVPIOJ-UHFFFAOYSA-N
Formula: C14H27NO4
SMILES: CCCOC(=O)N(C)CC(=O)OCCCC(C)C
Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
hf	-922.02	kJ/mol	Cheméo Relay (1.0)
hfus	37.09	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.74		Cheméo Relay (1.0)
logp	2.834		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
rinpol	1714.00		NIST Webbook
tb	573.06	K	Cheméo Relay (1.0)
tc	741.79	K	Cheméo Relay (1.0)
tf	240.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.75	J/mol×K	684.30	Joback Method
cpg	678.88	J/mol×K	713.88	Joback Method
cpg	694.21	J/mol×K	743.47	Joback Method
cpg	708.76	J/mol×K	773.05	Joback Method
cpg	722.52	J/mol×K	802.63	Joback Method
cpg	735.52	J/mol×K	832.22	Joback Method
cpg	747.76	J/mol×K	861.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320650&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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