

Glycine, N-methyl-N-propoxycarbonyl-, heptyl ester

Inchi:	InChI=1S/C14H27NO4/c1-4-6-7-8-9-11-18-13(16)12-15(3)14(17)19-10-5-2/h4-12H2,1-3H1
InchiKey:	LOMPIYIQMDGKSA-UHFFFAOYSA-N
Formula:	C14H27NO4
SMILES:	CCCCCCCCOC(=O)CN(C)C(=O)OCCCC
Mol. weight [g/mol]:	273.37

Physical Properties

Property code	Value	Unit	Source
hf	-904.54	kJ/mol	Cheméo Relay (1.0)
hfus	40.61	kJ/mol	Joback Method
hvap	83.64	kJ/mol	Cheméo Relay (1.0)
ie	8.88	eV	Cheméo Relay (1.0)
log10ws	-3.02		Cheméo Relay (1.0)
logp	2.978		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
tb	577.09	K	Cheméo Relay (1.0)
tc	748.86	K	Cheméo Relay (1.0)
tf	250.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.28	J/mol×K	684.74	Joback Method
cpg	678.19	J/mol×K	713.95	Joback Method
cpg	693.32	J/mol×K	743.17	Joback Method
cpg	707.69	J/mol×K	772.38	Joback Method
cpg	721.30	J/mol×K	801.60	Joback Method
cpg	734.18	J/mol×K	830.81	Joback Method
cpg	746.33	J/mol×K	860.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U320625&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ie:	Ionization energy
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
tf:	Normal melting (fusion) point

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