

Glycine, N-methyl-n-propoxycarbonyl-, undecyl ester

Inchi:	InChI=1S/C18H35NO4/c1-4-6-7-8-9-10-11-12-13-15-22-17(20)16-19(3)18(21)23-14-5-2/
InchiKey:	CYBJWILWEQTIHY-UHFFFAOYSA-N
Formula:	C18H35NO4
SMILES:	CCCCCCCCCCCCOC(=O)CN(C)C(=O)OCCC
Mol. weight [g/mol]:	329.47

Physical Properties

Property code	Value	Unit	Source
gf	-256.38	kJ/mol	Joback Method
hf	-836.92	kJ/mol	Joback Method
hfus	50.97	kJ/mol	Joback Method
hvap	76.02	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.539		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1225.98	kPa	Joback Method
rinsol	2104.00		NIST Webbook
tb	776.26	K	Joback Method
tc	955.77	K	Joback Method
tf	469.41	K	Joback Method
vc	1.109	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.02	J/molxK	776.26	Joback Method
cpg	909.60	J/molxK	806.18	Joback Method
cpg	926.22	J/molxK	836.10	Joback Method
cpg	941.90	J/molxK	866.02	Joback Method
cpg	956.65	J/molxK	895.93	Joback Method
cpg	970.50	J/molxK	925.85	Joback Method
cpg	983.46	J/molxK	955.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
gf:	Standard Gibbs free energy of formation
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
mccvol:	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
vc:	Critical Volume

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