

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

Inchi:	InChI=1S/C19H37NO4/c1-4-6-7-8-9-10-11-12-13-14-16-23-18(21)17-20(3)19(22)24-15-5
InchiKey:	HZFQQIFXNOKFNV-UHFFFAOYSA-N
Formula:	C19H37NO4
SMILES:	CCCCCCCCCCCCOC(=O)CN(C)C(=O)OCCC
Mol. weight [g/mol]:	343.50

Physical Properties

Property code	Value	Unit	Source
gf	-247.96	kJ/mol	Joback Method
hf	-857.56	kJ/mol	Joback Method
hfus	53.56	kJ/mol	Joback Method
hvap	78.24	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.929		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinsol	2183.00		NIST Webbook
tb	799.14	K	Joback Method
tc	981.27	K	Joback Method
tf	480.68	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.89	J/molxK	799.14	Joback Method
cpg	969.89	J/molxK	829.49	Joback Method
cpg	986.86	J/molxK	859.85	Joback Method
cpg	1002.84	J/molxK	890.20	Joback Method
cpg	1017.84	J/molxK	920.56	Joback Method
cpg	1031.88	J/molxK	950.91	Joback Method
cpg	1044.99	J/molxK	981.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320630&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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