

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

Inchi:

InChI=1S/C24H47NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-28-23(26)22-25

InchiKey:

DNXVMZMVYJTDAF-UHFFFAOYSA-N

Formula:

C24H47NO4

SMILES:

CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)OCCC

Mol. weight [g/mol]:

413.63

Physical Properties

Property code	Value	Unit	Source
gf	-205.86	kJ/mol	Joback Method
hf	-960.76	kJ/mol	Joback Method
hfus	66.51	kJ/mol	Joback Method
hvap	89.37	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.879		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	849.00	kPa	Joback Method
rinpol	2624.00		NIST Webbook
rinpol	2624.00		NIST Webbook
tb	913.54	K	Joback Method
tc	1121.26	K	Joback Method
tf	537.03	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1262.21	J/mol×K	913.54	Joback Method
cpg	1282.67	J/mol×K	948.16	Joback Method
cpg	1301.66	J/mol×K	982.78	Joback Method
cpg	1319.24	J/mol×K	1017.40	Joback Method
cpg	1335.44	J/mol×K	1052.02	Joback Method
cpg	1350.31	J/mol×K	1086.64	Joback Method
cpg	1363.91	J/mol×K	1121.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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