Glycine, N-methyl-N-ethoxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C23H45NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-28-22(25)21-24(
InchiKey: PBRDSJAWLZBCRZ-UHFFFAOYSA-N
Formula: C23H45NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)OCC
Mol. weight [g/mol]: 399.61

Physical Properties

Property code	Value	Unit	Source
gf	-214.28	kJ/mol	Joback Method
hf	-940.12	kJ/mol	Joback Method
hfus	63.92	kJ/mol	Joback Method
hvap	87.15	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.489		Crippen Method
mcvol	359.790	ml/mol	McGowan Method
pc	898.56	kPa	Joback Method
rinpol	2547.00		NIST Webbook
tb	890.66	K	Joback Method
tc	1091.36	K	Joback Method
tf	525.76	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1198.90	J/mol×K	890.66	Joback Method
cpg	1218.80	J/mol×K	924.11	Joback Method
cpg	1237.34	J/mol×K	957.56	Joback Method
cpg	1254.57	J/mol×K	991.01	Joback Method
cpg	1270.54	J/mol×K	1024.46	Joback Method
cpg	1285.26	J/mol×K	1057.91	Joback Method
cpg	1298.80	J/mol×K	1091.36	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=U320686&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume