Glycine, N-methyl-N-methoxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C22H43NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-27-21(24)20-23(2

InchiKey: AVHKKCBTBIKGFA-UHFFFAOYSA-N

Formula: C22H43NO4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)OC

Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
gf	-222.70	kJ/mol	Joback Method
hf	-919.48	kJ/mol	Joback Method
hfus	61.33	kJ/mol	Joback Method
hvap	84.92	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	6.099		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	952.60	kPa	Joback Method
rinpol	2512.00		NIST Webbook
tb	867.78	K	Joback Method
tc	1062.48	K	Joback Method
tf	514.49	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.15	J/mol×K	867.78	Joback Method
cpg	1155.53	J/mol×K	900.23	Joback Method
cpg	1173.65	J/mol×K	932.68	Joback Method
cpg	1190.55	J/mol×K	965.13	Joback Method
cpg	1206.27	J/mol×K	997.58	Joback Method
cpg	1220.84	J/mol×K	1030.03	Joback Method
cpg	1234.29	J/mol×K	1062.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U320616&Units=SI

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