

Glycine, N-methyl-N-methoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C21H41NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-26-20(23)19-22(2)21
InchiKey: XRJRABOQHOYWOL-UHFFFAOYSA-N
Formula: C21H41NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)OC
Mol. weight [g/mol]: 371.55

Physical Properties

Property code	Value	Unit	Source
gf	-231.12	kJ/mol	Joback Method
hf	-898.84	kJ/mol	Joback Method
hfus	58.74	kJ/mol	Joback Method
hvap	82.69	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.709		Crippen Method
mcvol	331.610	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	844.90	K	Joback Method
tc	1034.56	K	Joback Method
tf	503.22	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.03	J/mol×K	844.90	Joback Method
cpg	1092.91	J/mol×K	876.51	Joback Method
cpg	1110.63	J/mol×K	908.12	Joback Method
cpg	1127.22	J/mol×K	939.73	Joback Method
cpg	1142.70	J/mol×K	971.34	Joback Method
cpg	1157.10	J/mol×K	1002.95	Joback Method
cpg	1170.46	J/mol×K	1034.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinsol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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