

Glycine, N-capryloyl-, methyl ester

Inchi:	InChI=1S/C11H21NO3/c1-3-4-5-6-7-8-10(13)12-9-11(14)15-2/h3-9H2,1-2H3,(H,12,13)
InchiKey:	KJKMMCRBNDERQO-UHFFFAOYSA-N
Formula:	C11H21NO3
SMILES:	CCCCCCCC(=O)NCC(=O)OC
Mol. weight [g/mol]:	215.29

Physical Properties

Property code	Value	Unit	Source
gf	-231.71	kJ/mol	Joback Method
hf	-574.28	kJ/mol	Joback Method
hfus	33.73	kJ/mol	Joback Method
hvap	62.42	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.636		Crippen Method
mvol	184.840	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1664.00		NIST Webbook
rinpol	1664.00		NIST Webbook
tb	631.41	K	Joback Method
tc	812.70	K	Joback Method
tf	388.48	K	Joback Method
vc	0.717	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.13	J/molxK	631.41	Joback Method
cpg	506.14	J/molxK	661.63	Joback Method
cpg	519.50	J/molxK	691.84	Joback Method
cpg	532.20	J/molxK	722.06	Joback Method
cpg	544.27	J/molxK	752.27	Joback Method
cpg	555.70	J/molxK	782.49	Joback Method
cpg	566.52	J/molxK	812.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U299723&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
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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