

Glycine, N-methyl-N-allyloxycarbonyl-, decyl ester

Inchi:	InChI=1S/C17H31NO4/c1-4-6-7-8-9-10-11-12-14-21-16(19)15-18(3)17(20)22-13-5-2/h5H
InchiKey:	NWSIBZRURYAVMO-UHFFFAOYSA-N
Formula:	C17H31NO4
SMILES:	C=CCOC(=O)N(C)CC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	313.43

Physical Properties

Property code	Value	Unit	Source
gf	-176.96	kJ/mol	Joback Method
hf	-690.85	kJ/mol	Joback Method
hfus	47.10	kJ/mol	Joback Method
hvap	73.12	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.925		Crippen Method
mcvol	270.950	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	2008.00		NIST Webbook
tb	750.06	K	Joback Method
tc	928.70	K	Joback Method
tf	456.38	K	Joback Method
vc	1.034	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.52	J/mol×K	750.06	Joback Method
cpg	824.16	J/mol×K	779.83	Joback Method
cpg	839.92	J/mol×K	809.61	Joback Method
cpg	854.80	J/mol×K	839.38	Joback Method
cpg	868.84	J/mol×K	869.15	Joback Method
cpg	882.05	J/mol×K	898.92	Joback Method
cpg	894.44	J/mol×K	928.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.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
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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