

Glycine, N-methyl-N-allyloxycarbonyl-, nonyl ester

Inchi:	InChI=1S/C16H29NO4/c1-4-6-7-8-9-10-11-13-20-15(18)14-17(3)16(19)21-12-5-2/h5H,2,
InchiKey:	QSNLSJXSMSHQFD-UHFFFAOYSA-N
Formula:	C16H29NO4
SMILES:	C=CCOC(=O)N(C)CC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	299.41

Physical Properties

Property code	Value	Unit	Source
gf	-185.38	kJ/mol	Joback Method
hf	-670.21	kJ/mol	Joback Method
hfus	44.51	kJ/mol	Joback Method
hvap	70.89	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.535		Crippen Method
mvol	256.860	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tb	727.18	K	Joback Method
tc	904.82	K	Joback Method
tf	445.11	K	Joback Method
vc	0.979	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.13	J/molxK	727.18	Joback Method
cpg	766.37	J/molxK	756.79	Joback Method
cpg	781.76	J/molxK	786.39	Joback Method
cpg	796.33	J/molxK	816.00	Joback Method
cpg	810.09	J/molxK	845.61	Joback Method
cpg	823.05	J/molxK	875.21	Joback Method
cpg	835.24	J/molxK	904.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320593&Units=SI
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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