

Glycine, N-methyl-N-butoxycarbonyl-, nonyl ester

Inchi:	InChI=1S/C17H33NO4/c1-4-6-8-9-10-11-12-14-21-16(19)15-18(3)17(20)22-13-7-5-2/h4-17
InchiKey:	WZVNSIHNENTGPT-UHFFFAOYSA-N
Formula:	C17H33NO4
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)OCCCC
Mol. weight [g/mol]:	315.45

Physical Properties

Property code	Value	Unit	Source
af	0.9636		Cheméo Relay (1.0)
hf	-964.37	kJ/mol	Cheméo Relay (1.0)
hfus	48.38	kJ/mol	Joback Method
hvap	97.05	kJ/mol	Cheméo Relay (1.0)
ie	8.88	eV	Cheméo Relay (1.0)
log10ws	-4.09		Cheméo Relay (1.0)
logp	4.149		Crippen Method
mcvol	275.250	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	2007.00		NIST Webbook
rinpol	2007.00		NIST Webbook
tb	597.84	K	Cheméo Relay (1.0)
tc	780.02	K	Cheméo Relay (1.0)
tf	262.28	K	Cheméo Relay (1.0)
vc	1.066	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.05	J/mol×K	753.38	Joback Method
cpg	850.22	J/mol×K	782.98	Joback Method
cpg	866.48	J/mol×K	812.57	Joback Method
cpg	881.85	J/mol×K	842.17	Joback Method
cpg	896.35	J/mol×K	871.76	Joback Method
cpg	909.99	J/mol×K	901.36	Joback Method
cpg	922.78	J/mol×K	930.96	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320654&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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