

Glycine, N-methyl-N-butoxycarbonyl-, pentyl ester

Inchi:	InChI=1S/C13H25NO4/c1-4-6-8-10-17-12(15)11-14(3)13(16)18-9-7-5-2/h4-11H2,1-3H3
InchiKey:	YLTXWCDIDPJYQF-UHFFFAOYSA-N
Formula:	C13H25NO4
SMILES:	CCCCCOC(=O)CN(C)C(=O)OCCCC
Mol. weight [g/mol]:	259.35

Physical Properties

Property code	Value	Unit	Source
af	0.8207		Cheméo Relay (1.0)
hf	-888.47	kJ/mol	Cheméo Relay (1.0)
hfus	38.02	kJ/mol	Joback Method
hvap	82.34	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-2.53		Cheméo Relay (1.0)
logp	2.588		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
tb	565.26	K	Cheméo Relay (1.0)
tc	740.00	K	Cheméo Relay (1.0)
tf	240.65	K	Cheméo Relay (1.0)
vc	0.846	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.70	J/mol×K	661.86	Joback Method
cpg	623.13	J/mol×K	691.11	Joback Method
cpg	637.83	J/mol×K	720.36	Joback Method
cpg	651.80	J/mol×K	749.62	Joback Method
cpg	665.07	J/mol×K	778.87	Joback Method
cpg	677.63	J/mol×K	808.12	Joback Method
cpg	689.49	J/mol×K	837.37	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320649&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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