

Glycine, N-methyl-n-propoxycarbonyl-, butyl ester

Inchi:	InChI=1S/C11H21NO4/c1-4-6-8-15-10(13)9-12(3)11(14)16-7-5-2/h4-9H2,1-3H3
InchiKey:	JUVYDHZBIGUSND-UHFFFAOYSA-N
Formula:	C11H21NO4
SMILES:	CCCCOC(=O)CN(C)C(=O)OCCC
Mol. weight [g/mol]:	231.29

Physical Properties

Property code	Value	Unit	Source
gf	-315.32	kJ/mol	Joback Method
hf	-692.44	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	60.44	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.808		Crippen Method
mcvol	190.710	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
tb	616.10	K	Joback Method
tc	793.24	K	Joback Method
tf	390.52	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.57	J/molxK	616.10	Joback Method
cpg	516.91	J/molxK	645.62	Joback Method
cpg	530.61	J/molxK	675.15	Joback Method
cpg	543.66	J/molxK	704.67	Joback Method
cpg	556.07	J/molxK	734.19	Joback Method
cpg	567.86	J/molxK	763.72	Joback Method
cpg	579.01	J/molxK	793.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320621&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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