

Sarcosylsarcosine, n-propoxycarbonyl-, ethyl ester

Inchi:	InChI=1S/C12H22N2O5/c1-5-7-19-12(17)14(4)8-10(15)13(3)9-11(16)18-6-2/h5-9H2,1-4H
InchiKey:	YSLQSDMVJFCZJA-UHFFFAOYSA-N
Formula:	C12H22N2O5
SMILES:	CCCOC(=O)N(C)CC(=O)N(C)CC(=O)OCC
Mol. weight [g/mol]:	274.31

Physical Properties

Property code	Value	Unit	Source
gf	-325.04	kJ/mol	Joback Method
hf	-758.13	kJ/mol	Joback Method
hfus	40.05	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-0.46		Crippen Method
logp	0.486		Crippen Method
mcvol	216.350	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1995.00		NIST Webbook
tb	705.29	K	Joback Method
tc	888.00	K	Joback Method
tf	484.19	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.69	J/mol×K	705.29	Joback Method
cpg	628.69	J/mol×K	735.74	Joback Method
cpg	641.90	J/mol×K	766.19	Joback Method
cpg	654.35	J/mol×K	796.64	Joback Method
cpg	666.03	J/mol×K	827.10	Joback Method
cpg	676.96	J/mol×K	857.55	Joback Method
cpg	687.16	J/mol×K	888.00	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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