

Sarcosylsarcosine, N-ethoxycarbonyl-, ethyl ester

Inchi:	InChI=1S/C11H20N2O5/c1-5-17-10(15)8-12(3)9(14)7-13(4)11(16)18-6-2/h5-8H2,1-4H3
InchiKey:	NLFBMJHGPSCLRP-UHFFFAOYSA-N
Formula:	C11H20N2O5
SMILES:	CCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC
Mol. weight [g/mol]:	260.29

Physical Properties

Property code	Value	Unit	Source
gf	-333.46	kJ/mol	Joback Method
hf	-737.49	kJ/mol	Joback Method
hfus	37.46	kJ/mol	Joback Method
hvap	69.22	kJ/mol	Joback Method
log10ws	-0.05		Crippen Method
logp	0.096		Crippen Method
mcvol	202.260	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinsol	1908.00		NIST Webbook
tb	682.41	K	Joback Method
tc	865.77	K	Joback Method
tf	472.92	K	Joback Method
vc	0.742	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.29	J/mol×K	682.41	Joback Method
cpg	574.82	J/mol×K	712.97	Joback Method
cpg	587.60	J/mol×K	743.53	Joback Method
cpg	599.65	J/mol×K	774.09	Joback Method
cpg	610.98	J/mol×K	804.65	Joback Method
cpg	621.59	J/mol×K	835.21	Joback Method
cpg	631.50	J/mol×K	865.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320688&Units=SI

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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