

Sarcosylsarcosine, N-butoxycarbonyl-, ethyl ester

Inchi:	InChI=1S/C13H24N2O5/c1-5-7-8-20-13(18)15(4)9-11(16)14(3)10-12(17)19-6-2/h5-10H2
InchiKey:	QVZQUFYQCBARQY-UHFFFAOYSA-N
Formula:	C13H24N2O5
SMILES:	CCCCOC(=O)N(C)CC(=O)N(C)CC(=O)OCC
Mol. weight [g/mol]:	288.34

Physical Properties

Property code	Value	Unit	Source
af	0.8413		Cheméo Relay (1.0)
hf	-984.94	kJ/mol	Cheméo Relay (1.0)
hfus	42.64	kJ/mol	Joback Method
hvap	87.20	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-1.01		Cheméo Relay (1.0)
logp	0.876		Crippen Method
mcvol	230.440	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
rinpol	2072.00		NIST Webbook
tb	577.57	K	Cheméo Relay (1.0)
tc	765.47	K	Cheméo Relay (1.0)
tf	285.24	K	Cheméo Relay (1.0)
vc	0.880	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.30	J/mol×K	728.17	Joback Method
cpg	683.73	J/mol×K	758.59	Joback Method
cpg	697.33	J/mol×K	789.02	Joback Method
cpg	710.12	J/mol×K	819.44	Joback Method
cpg	722.11	J/mol×K	849.86	Joback Method
cpg	733.33	J/mol×K	880.28	Joback Method
cpg	743.77	J/mol×K	910.71	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320663&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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