

Sarcosylsarcosine, n-butoxycarbonyl-, butyl ester

Inchi:	InChI=1S/C15H28N2O5/c1-5-7-9-21-14(19)12-16(3)13(18)11-17(4)15(20)22-10-8-6-2/h5
InchiKey:	LIFSRIBRQMAORB-UHFFFAOYSA-N
Formula:	C15H28N2O5
SMILES:	CCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCCCC
Mol. weight [g/mol]:	316.39

Physical Properties

Property code	Value	Unit	Source
gf	-299.78	kJ/mol	Joback Method
hf	-820.05	kJ/mol	Joback Method
hfus	47.82	kJ/mol	Joback Method
hvap	78.13	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.657		Crippen Method
mcvol	258.620	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
tb	773.93	K	Joback Method
tc	957.76	K	Joback Method
tf	518.00	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.78	J/mol×K	773.93	Joback Method
cpg	796.98	J/mol×K	804.57	Joback Method
cpg	811.28	J/mol×K	835.21	Joback Method
cpg	824.68	J/mol×K	865.84	Joback Method
cpg	837.21	J/mol×K	896.48	Joback Method
cpg	848.88	J/mol×K	927.12	Joback Method
cpg	859.71	J/mol×K	957.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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