

Sarcosylsarcosine, n-butoxycarbonyl-, nonyl ester

Inchi: InChI=1S/C20H38N2O5/c1-5-7-9-10-11-12-13-15-26-19(24)17-21(3)18(23)16-22(4)20(25)2
InchiKey: SWLRAGNGCSRCLV-UHFFFAOYSA-N
Formula: C20H38N2O5
SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCCCC
Mol. weight [g/mol]: 386.53

Physical Properties

Property code	Value	Unit	Source
gf	-257.68	kJ/mol	Joback Method
hf	-923.25	kJ/mol	Joback Method
hfus	60.77	kJ/mol	Joback Method
hvap	89.26	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.607		Crippen Method
mcvol	329.070	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2647.00		NIST Webbook
tb	888.33	K	Joback Method
tc	1087.57	K	Joback Method
tf	574.35	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.44	J/mol×K	888.33	Joback Method
cpg	1095.57	J/mol×K	921.54	Joback Method
cpg	1111.48	J/mol×K	954.74	Joback Method
cpg	1126.21	J/mol×K	987.95	Joback Method
cpg	1139.78	J/mol×K	1021.15	Joback Method
cpg	1152.23	J/mol×K	1054.36	Joback Method
cpg	1163.60	J/mol×K	1087.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320669&Units=SI
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

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

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