

Sarcosylsarcosine, n-butoxycarbonyl-, octyl ester

Inchi: InChI=1S/C19H36N2O5/c1-5-7-9-10-11-12-14-25-18(23)16-20(3)17(22)15-21(4)19(24)20(25)26-13-2
InchiKey: CHKDOOKXTALEFT-UHFFFAOYSA-N
Formula: C19H36N2O5
SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCCCC
Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
gf	-266.10	kJ/mol	Joback Method
hf	-902.61	kJ/mol	Joback Method
hfus	58.18	kJ/mol	Joback Method
hvap	87.03	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.217		Crippen Method
mcvol	314.980	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2556.00		NIST Webbook
tb	865.45	K	Joback Method
tc	1059.97	K	Joback Method
tf	563.08	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.62	J/mol×K	865.45	Joback Method
cpg	1034.34	J/mol×K	897.87	Joback Method
cpg	1049.91	J/mol×K	930.29	Joback Method
cpg	1064.38	J/mol×K	962.71	Joback Method
cpg	1077.75	J/mol×K	995.13	Joback Method
cpg	1090.08	J/mol×K	1027.55	Joback Method
cpg	1101.39	J/mol×K	1059.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320668&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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