

Sarcosylsarcosine, N-isobutoxycarbonyl-, nonyl ester

Inchi:	InChI=1S/C20H38N2O5/c1-6-7-8-9-10-11-12-13-26-19(24)15-21(4)18(23)14-22(5)20(25)
InchiKey:	UICZUHRSGMBOOA-UHFFFAOYSA-N
Formula:	C20H38N2O5
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC(C)C
Mol. weight [g/mol]:	386.53

Physical Properties

Property code	Value	Unit	Source
gf	-260.12	kJ/mol	Joback Method
hf	-928.53	kJ/mol	Joback Method
hfus	57.25	kJ/mol	Joback Method
hvap	88.87	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.463		Crippen Method
mcvol	329.070	ml/mol	McGowan Method
pc	1126.83	kPa	Joback Method
rinpol	2592.00		NIST Webbook
tb	887.89	K	Joback Method
tc	1087.08	K	Joback Method
tf	559.35	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.90	J/molxK	887.89	Joback Method
cpg	1096.01	J/molxK	921.09	Joback Method
cpg	1111.89	J/molxK	954.29	Joback Method
cpg	1126.57	J/molxK	987.48	Joback Method
cpg	1140.09	J/molxK	1020.68	Joback Method
cpg	1152.48	J/molxK	1053.88	Joback Method
cpg	1163.78	J/molxK	1087.08	Joback Method

Sources

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=U320584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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