

Sarcosylsarcosine, N-isobutoxycarbonyl-, octyl ester

Inchi:	InChI=1S/C19H36N2O5/c1-6-7-8-9-10-11-12-25-18(23)14-20(4)17(22)13-21(5)19(24)26
InchiKey:	CKROKXBFSPNKF-UHFFFAOYSA-N
Formula:	C19H36N2O5
SMILES:	CCCCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC(C)C
Mol. weight [g/mol]:	372.50

Physical Properties

Property code	Value	Unit	Source
gf	-268.54	kJ/mol	Joback Method
hf	-907.89	kJ/mol	Joback Method
hfus	54.66	kJ/mol	Joback Method
hvap	86.64	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	3.073		Crippen Method
mvol	314.980	ml/mol	McGowan Method
pc	1203.12	kPa	Joback Method
rinpol	2508.00		NIST Webbook
rinpol	2508.00		NIST Webbook
tb	865.01	K	Joback Method
tc	1059.84	K	Joback Method
tf	548.08	K	Joback Method
vc	1.183	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1018.10	J/mol×K	865.01	Joback Method
cpg	1034.84	J/mol×K	897.48	Joback Method
cpg	1050.41	J/mol×K	929.95	Joback Method
cpg	1064.86	J/mol×K	962.42	Joback Method
cpg	1078.21	J/mol×K	994.90	Joback Method
cpg	1090.49	J/mol×K	1027.37	Joback Method
cpg	1101.75	J/mol×K	1059.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=U320583&Units=SI

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

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