Sarcosylsarcosine, N-isobutoxycarbonyl-, ethyl ester

Inchi: InChI=1S/C13H24N2O5/c1-6-19-12(17)8-14(4)11(16)7-15(5)13(18)20-9-10(2)3/h10H,6-9

InchiKey: CUQIPAIAUGJIRY-UHFFFAOYSA-N

Formula: C13H24N2O5

SMILES: CCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC(C)C

Mol. weight [g/mol]: 288.34

Physical Properties

Property code	Value	Unit	Source
gf	-319.06	kJ/mol	Joback Method
hf	-784.05	kJ/mol	Joback Method
hfus	39.12	kJ/mol	Joback Method
hvap	73.29	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.732		Crippen Method
mcvol	230.440	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	2027.00		NIST Webbook
tb	727.73	K	Joback Method
tc	912.40	K	Joback Method
tf	480.46	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.83	J/mol×K	727.73	Joback Method
cpg	684.44	J/mol×K	758.51	Joback Method
cpg	698.20	J/mol×K	789.29	Joback Method
cpg	711.12	J/mol×K	820.07	Joback Method
cpg	723.22	J/mol×K	850.85	Joback Method
cpg	734.51	J/mol×K	881.62	Joback Method
cpg	745.01	J/mol×K	912.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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