

Sarcosylsarcosine, N-isobutoxycarbonyl-, decyl ester

Inchi:	InChI=1S/C21H40N2O5/c1-6-7-8-9-10-11-12-13-14-27-20(25)16-22(4)19(24)15-23(5)21
InchiKey:	BMHSXUKIEMWTRR-UHFFFAOYSA-N
Formula:	C21H40N2O5
SMILES:	CCCCCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC(C)C
Mol. weight [g/mol]:	400.55

Physical Properties

Property code	Value	Unit	Source
gf	-251.70	kJ/mol	Joback Method
hf	-949.17	kJ/mol	Joback Method
hfus	59.84	kJ/mol	Joback Method
hvap	91.10	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.853		Crippen Method
mcvol	343.160	ml/mol	McGowan Method
pc	1057.57	kPa	Joback Method
rinpol	2684.00		NIST Webbook
rinpol	2684.00		NIST Webbook
tb	910.77	K	Joback Method
tc	1115.25	K	Joback Method
tf	570.62	K	Joback Method
vc	1.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1140.31	J/molxK	910.77	Joback Method
cpg	1157.83	J/molxK	944.85	Joback Method
cpg	1174.02	J/molxK	978.93	Joback Method
cpg	1188.94	J/molxK	1013.01	Joback Method
cpg	1202.62	J/molxK	1047.09	Joback Method
cpg	1215.10	J/molxK	1081.17	Joback Method
cpg	1226.42	J/molxK	1115.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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