Sarcosylsarcosine, n-butoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C18H34N2O5/c1-5-7-9-10-11-13-24-17(22)15-19(3)16(21)14-20(4)18(23)25-12

InchiKey: SFXXNTNGJDEVJC-UHFFFAOYSA-N

Formula: C18H34N2O5

SMILES: CCCCCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCCCC

Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-274.52	kJ/mol	Joback Method
hf	-881.97	kJ/mol	Joback Method
hfus	55.59	kJ/mol	Joback Method
hvap	84.81	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.827		Crippen Method
mcvol	300.890	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2478.00		NIST Webbook
rinpol	2478.00		NIST Webbook
tb	842.57	K	Joback Method
tc	1033.26	K	Joback Method
tf	551.81	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.48	J/mol×K	842.57	Joback Method
cpg	973.80	J/mol×K	874.35	Joback Method
cpg	989.06	J/mol×K	906.13	Joback Method
cpg	1003.26	J/mol×K	937.91	Joback Method
cpg	1016.44	J/mol×K	969.69	Joback Method
cpg	1028.62	J/mol×K	1001.47	Joback Method
cpg	1039.84	J/mol×K	1033.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320667&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

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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