Sarcosylsarcosine, N-ethoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C16H30N2O5/c1-5-7-8-9-10-11-23-15(20)13-17(3)14(19)12-18(4)16(21)22-6-2

InchiKey: FWKKHJWBIPQUCJ-UHFFFAOYSA-N

Formula: C16H30N2O5

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

Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-291.36	kJ/mol	Joback Method
hf	-840.69	kJ/mol	Joback Method
hfus	50.41	kJ/mol	Joback Method
hvap	80.35	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.047		Crippen Method
mcvol	272.710	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2319.00		NIST Webbook
tb	796.81	K	Joback Method
tc	982.21	K	Joback Method
tf	529.27	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.49	J/mol×K	796.81	Joback Method
cpg	855.06	J/mol×K	827.71	Joback Method
cpg	869.68	J/mol×K	858.61	Joback Method
cpg	883.36	J/mol×K	889.51	Joback Method
cpg	896.12	J/mol×K	920.41	Joback Method
cpg	907.98	J/mol×K	951.31	Joback Method
cpg	918.96	J/mol×K	982.21	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=U320693&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