Sarcosine, N-valeryl-, undecyl ester

Inchi: InChI=1S/C19H37NO3/c1-4-6-8-9-10-11-12-13-14-16-23-19(22)17-20(3)18(21)15-7-5-2/l
InchiKey: HTVWMCMFIIJGGG-UHFFFAOYSA-N
Formula: C19H37NO3
SMILES: CCCCCCCCCCCOC(=O)CN(C)C(=O)CCCC
Mol. weight [g/mol]: 327.50

Physical Properties

Property code	Value	Unit	Source
gf	-142.96	kJ/mol	Joback Method
hf	-725.34	kJ/mol	Joback Method
hfus	52.37	kJ/mol	Joback Method
hvap	75.83	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.709		Crippen Method
mcvol	297.560	ml/mol	McGowan Method
pc	1160.87	kPa	Joback Method
rinpol	2407.00		NIST Webbook
rinpol	2407.00		NIST Webbook
tb	776.72	K	Joback Method
tc	956.01	K	Joback Method
tf	458.45	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.24	J/mol×K	776.72	Joback Method
cpg	938.43	J/mol×K	806.60	Joback Method
cpg	955.66	J/mol×K	836.48	Joback Method
cpg	971.95	J/mol×K	866.36	Joback Method
cpg	987.33	J/mol×K	896.24	Joback Method
cpg	1001.84	J/mol×K	926.13	Joback Method
cpg	1015.50	J/mol×K	956.01	Joback Method

Sources

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=U321566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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