Sarcosine, N-hexanoyl-, propyl ester

Inchi: InChI=1S/C12H23NO3/c1-4-6-7-8-11(14)13(3)10-12(15)16-9-5-2/h4-10H2,1-3H3
InchiKey: LQFIURSLIIRQRX-UHFFFAOYSA-N
Formula: C12H23NO3
SMILES: CCCCCC(=O)N(C)CC(=O)OCCC
Mol. weight [g/mol]: 229.32

Physical Properties

Property code	Value	Unit	Source
hf	-699.01	kJ/mol	Cheméo Relay (1.0)
hfus	34.24	kJ/mol	Joback Method
hvap	72.01	kJ/mol	Cheméo Relay (1.0)
ie	8.67	eV	Cheméo Relay (1.0)
log10ws	-1.67		Cheméo Relay (1.0)
logp	1.978		Crippen Method
mcvol	198.930	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1715.00		NIST Webbook
rinpol	1715.00		NIST Webbook
tb	548.53	K	Cheméo Relay (1.0)
tc	722.53	K	Cheméo Relay (1.0)
tf	256.75	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.69	J/mol×K	616.56	Joback Method
cpg	541.82	J/mol×K	645.96	Joback Method
cpg	556.25	J/mol×K	675.37	Joback Method
cpg	569.98	J/mol×K	704.77	Joback Method
cpg	583.05	J/mol×K	734.17	Joback Method
cpg	595.45	J/mol×K	763.58	Joback Method
cpg	607.21	J/mol×K	792.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321123&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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