Sarcosine, N-hexanoyl-, octyl ester

Inchi: InChI=1S/C17H33NO3/c1-4-6-8-9-10-12-14-21-17(20)15-18(3)16(19)13-11-7-5-2/h4-15H
InchiKey: ZXWZUZMQURKFNG-UHFFFAOYSA-N
Formula: C17H33NO3
SMILES: CCCCCCCCOC(=O)CN(C)C(=O)CCCCC
Mol. weight [g/mol]: 299.45

Physical Properties

Property code	Value	Unit	Source
hf	-799.75	kJ/mol	Cheméo Relay (1.0)
hfus	47.19	kJ/mol	Joback Method
hvap	90.55	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.60		Cheméo Relay (1.0)
logp	3.929		Crippen Method
mcvol	269.380	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpol	2197.00		NIST Webbook
tb	591.81	K	Cheméo Relay (1.0)
tc	778.02	K	Cheméo Relay (1.0)
tf	279.33	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.22	J/mol×K	730.96	Joback Method
cpg	819.60	J/mol×K	760.27	Joback Method
cpg	836.10	J/mol×K	789.59	Joback Method
cpg	851.75	J/mol×K	818.90	Joback Method
cpg	866.57	J/mol×K	848.21	Joback Method
cpg	880.59	J/mol×K	877.53	Joback Method
cpg	893.82	J/mol×K	906.84	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321126&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

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
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