Sarcosine, N-hexanoyl-, octadecyl ester

Inchi: InChI=1S/C27H53NO3/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-22-24-31-27(30)25
InchiKey: OALXXRCTXZBODD-UHFFFAOYSA-N
Formula: C27H53NO3
SMILES: CCCCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCCC
Mol. weight [g/mol]: 439.72

Physical Properties

Property code	Value	Unit	Source
hf	-1004.13	kJ/mol	Cheméo Relay (1.0)
hfus	73.09	kJ/mol	Joback Method
hvap	129.90	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.89		Cheméo Relay (1.0)
logp	7.830		Crippen Method
mcvol	410.280	ml/mol	McGowan Method
pc	729.28	kPa	Joback Method
tb	659.03	K	Cheméo Relay (1.0)
tc	852.62	K	Cheméo Relay (1.0)
tf	318.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1422.59	J/mol×K	959.76	Joback Method
cpg	1445.34	J/mol×K	997.40	Joback Method
cpg	1466.43	J/mol×K	1035.03	Joback Method
cpg	1485.94	J/mol×K	1072.67	Joback Method
cpg	1503.97	J/mol×K	1110.30	Joback Method
cpg	1520.59	J/mol×K	1147.94	Joback Method
cpg	1535.90	J/mol×K	1185.58	Joback Method

Sources

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=U321133&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point