

Sarcosine, n-hexanoyl-, heptadecyl ester

Inchi:	InChI=1S/C26H51NO3/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-21-23-30-26(29)24-27
InchiKey:	WWKUJGWIUXURRB-UHFFFAOYSA-N
Formula:	C26H51NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCCC
Mol. weight [g/mol]:	425.69

Physical Properties

Property code	Value	Unit	Source
gf	-84.02	kJ/mol	Joback Method
hf	-869.82	kJ/mol	Joback Method
hfus	70.50	kJ/mol	Joback Method
hvap	91.42	kJ/mol	Joback Method
log10ws	-7.91		Crippen Method
logp	7.440		Crippen Method
mcvol	396.190	ml/mol	McGowan Method
pc	768.61	kPa	Joback Method
tb	936.88	K	Joback Method
tc	1153.23	K	Joback Method
tf	537.34	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1357.77	J/molxK	936.88	Joback Method
cpg	1379.76	J/molxK	972.94	Joback Method
cpg	1400.23	J/molxK	1009.00	Joback Method
cpg	1419.24	J/molxK	1045.05	Joback Method
cpg	1436.86	J/molxK	1081.11	Joback Method
cpg	1453.18	J/molxK	1117.17	Joback Method
cpg	1468.27	J/molxK	1153.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321132&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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