

Sarcosine, n-hexanoyl-, tetradecyl ester

Inchi:	InChI=1S/C23H45NO3/c1-4-6-8-9-10-11-12-13-14-15-16-18-20-27-23(26)21-24(3)22(25)
InchiKey:	JSNCELRYACBTPO-UHFFFAOYSA-N
Formula:	C23H45NO3
SMILES:	CCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCCC
Mol. weight [g/mol]:	383.61

Physical Properties

Property code	Value	Unit	Source
gf	-109.28	kJ/mol	Joback Method
hf	-807.90	kJ/mol	Joback Method
hfus	62.73	kJ/mol	Joback Method
hvap	84.74	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	6.269		Crippen Method
mvol	353.920	ml/mol	McGowan Method
pc	907.79	kPa	Joback Method
rinpol	2829.00		NIST Webbook
rinpol	2829.00		NIST Webbook
tb	868.24	K	Joback Method
tc	1063.09	K	Joback Method
tf	503.53	K	Joback Method
vc	1.371	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1166.36	J/molxK	868.24	Joback Method
cpg	1186.44	J/molxK	900.72	Joback Method
cpg	1205.31	J/molxK	933.19	Joback Method
cpg	1223.00	J/molxK	965.67	Joback Method
cpg	1239.57	J/molxK	998.14	Joback Method
cpg	1255.06	J/molxK	1030.62	Joback Method
cpg	1269.52	J/molxK	1063.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321129&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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