

Sarcosine, N-(3-phenylpropionyl)-, tetradecyl ester

Inchi:	InChI=1S/C26H43NO3/c1-3-4-5-6-7-8-9-10-11-12-13-17-22-30-26(29)23-27(2)25(28)21-
InchiKey:	MSTSIIPKJANIEB-UHFFFAOYSA-N
Formula:	C26H43NO3
SMILES:	CCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCc1ccccc1
Mol. weight [g/mol]:	417.62

Physical Properties

Property code	Value	Unit	Source
gf	28.39	kJ/mol	Joback Method
hf	-633.29	kJ/mol	Joback Method
hfus	64.54	kJ/mol	Joback Method
hvap	93.69	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	6.322		Crippen Method
mcvol	372.430	ml/mol	McGowan Method
pc	931.78	kPa	Joback Method
tb	963.56	K	Joback Method
tc	1179.92	K	Joback Method
tf	563.76	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1258.09	J/molxK	963.56	Joback Method
cpg	1276.55	J/molxK	999.62	Joback Method
cpg	1293.65	J/molxK	1035.68	Joback Method
cpg	1309.48	J/molxK	1071.74	Joback Method
cpg	1324.11	J/molxK	1107.80	Joback Method
cpg	1337.63	J/molxK	1143.86	Joback Method
cpg	1350.11	J/molxK	1179.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321418&Units=SI

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

Latest version available from:

<https://www.chemeo.com/cid/40-573-1/Sarcosine-N-3-phenylpropionyl-tetradecyl-ester.pdf>

Generated by Cheméo on 2024-04-26 06:16:07.444487997 +0000 UTC m=+16401416.365065313.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.