Sarcosine, N-(3-fluorobenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C26H42FNO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-31-25(29)22-28(2)26
InchiKey: WURHZBUGJVDQPD-UHFFFAOYSA-N
Formula: C26H42FNO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 435.62

Physical Properties

Property code	Value	Unit	Source
gf	-176.05	kJ/mol	Joback Method
hf	-840.87	kJ/mol	Joback Method
hfus	67.23	kJ/mol	Joback Method
hvap	93.54	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.922		Crippen Method
mcvol	374.200	ml/mol	McGowan Method
pc	898.56	kPa	Joback Method
tb	967.81	K	Joback Method
tc	1186.20	K	Joback Method
tf	576.87	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1264.50	J/mol×K	967.81	Joback Method
cpg	1282.81	J/mol×K	1004.21	Joback Method
cpg	1299.73	J/mol×K	1040.61	Joback Method
cpg	1315.33	J/mol×K	1077.01	Joback Method
cpg	1329.70	J/mol×K	1113.41	Joback Method
cpg	1342.91	J/mol×K	1149.81	Joback Method
cpg	1355.04	J/mol×K	1186.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol:	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/66-452-7/Sarcosine-N-3-fluorobenzoyl-hexadecyl-ester.pdf

Generated by Cheméo on 2024-04-27 15:10:07.122781537 +0000 UTC m=+16519856.043358856.

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