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

Inchi: InChI=1S/C24H38FNO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-18-29-23(27)20-26(2)24(28)21

InchiKey: PTGUWKXTSMBJLI-UHFFFAOYSA-N

Formula: C24H38FNO3

SMILES: CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(F)c1

Mol. weight [g/mol]: 407.56

Physical Properties

Property code	Value	Unit	Source
gf	-192.89	kJ/mol	Joback Method
hf	-799.59	kJ/mol	Joback Method
hfus	62.05	kJ/mol	Joback Method
hvap	89.08	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.142		Crippen Method
mcvol	346.020	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	3081.00		NIST Webbook
rinpol	3081.00		NIST Webbook
tb	922.05	K	Joback Method
tc	1128.93	K	Joback Method
tf	554.33	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.86	J/mol×K	922.05	Joback Method
cpg	1157.33	J/mol×K	956.53	Joback Method
cpg	1173.55	J/mol×K	991.01	Joback Method
cpg	1188.59	J/mol×K	1025.49	Joback Method
cpg	1202.51	J/mol×K	1059.97	Joback Method
cpg	1215.36	J/mol×K	1094.45	Joback Method
cpg	1227.21	J/mol×K	1128.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321395&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
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/64-649-1/Sarcosine-N-3-fluorobenzoyl-tetradecyl-ester.pdf

Generated by Cheméo on 2024-04-29 01:54:24.786752231 +0000 UTC m=+16644913.707329546.

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