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]: 407.57

Physical Properties

Property code	Value	Unit	Source
hfus	62.05	kJ/mol	Joback Method
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-6.62		Cheméo Relay (1.0)
logp	6.142		Crippen Method
mcvol	346.020	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	3081.00		NIST Webbook
tb	670.65	K	Cheméo Relay (1.0)
tf	312.48	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321395&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point