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

Inchi: InChI=1S/C22H34FNO3/c1-3-4-5-6-7-8-9-10-11-12-16-27-21(25)18-24(2)22(26)19-14-13
InchiKey: AINQNEMXMVMICA-UHFFFAOYSA-N
Formula: C22H34FNO3
SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 379.51

Physical Properties

Property code	Value	Unit	Source
gf	-209.73	kJ/mol	Joback Method
hf	-758.31	kJ/mol	Joback Method
hfus	56.87	kJ/mol	Joback Method
hvap	84.63	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.362		Crippen Method
mcvol	317.840	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook
tb	876.29	K	Joback Method
tc	1075.53	K	Joback Method
tf	531.79	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.51	J/mol×K	876.29	Joback Method
cpg	1034.28	J/mol×K	909.50	Joback Method
cpg	1049.93	J/mol×K	942.70	Joback Method
cpg	1064.49	J/mol×K	975.91	Joback Method
cpg	1078.01	J/mol×K	1009.11	Joback Method
cpg	1090.55	J/mol×K	1042.32	Joback Method
cpg	1102.15	J/mol×K	1075.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321394&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

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