Sarcosine, N-(2,3,4-trifluorobenzoyl)-, heptadecyl ester

Inchi: InChI=1S/C27H42F3NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-34-24(32)21-31(
InchiKey: LHCIXFJJELZQPE-UHFFFAOYSA-N
Formula: C27H42F3NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 485.62

Physical Properties

Property code	Value	Unit	Source
gf	-576.51	kJ/mol	Joback Method
hf	-1276.67	kJ/mol	Joback Method
hfus	75.21	kJ/mol	Joback Method
hvap	95.45	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	7.591		Crippen Method
mcvol	391.830	ml/mol	McGowan Method
pc	792.60	kPa	Joback Method
tb	999.19	K	Joback Method
tc	1233.85	K	Joback Method
tf	614.36	K	Joback Method
vc	1.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1340.01	J/mol×K	999.19	Joback Method
cpg	1358.80	J/mol×K	1038.30	Joback Method
cpg	1375.96	J/mol×K	1077.41	Joback Method
cpg	1391.58	J/mol×K	1116.52	Joback Method
cpg	1405.73	J/mol×K	1155.63	Joback Method
cpg	1418.51	J/mol×K	1194.74	Joback Method
cpg	1430.00	J/mol×K	1233.85	Joback Method

Sources

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=U321488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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