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

Inchi: InChI=1S/C25H38F3NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-32-22(30)19-29(2)25(3

InchiKey: ZLURZNPOFKXDHP-UHFFFAOYSA-N

Formula: C25H38F3NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 457.57

Physical Properties

Property code	Value	Unit	Source
gf	-593.35	kJ/mol	Joback Method
hf	-1235.39	kJ/mol	Joback Method
hfus	70.03	kJ/mol	Joback Method
hvap	91.00	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	6.810		Crippen Method
mcvol	363.650	ml/mol	McGowan Method
pc	885.77	kPa	Joback Method
rinpol	3127.00		NIST Webbook
rinpol	3127.00		NIST Webbook
tb	953.43	K	Joback Method
tc	1170.27	K	Joback Method
tf	591.82	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1214.77	J/mol×K	953.43	Joback Method
cpg	1232.41	J/mol×K	989.57	Joback Method
cpg	1248.65	J/mol×K	1025.71	Joback Method
cpg	1263.57	J/mol×K	1061.85	Joback Method
cpg	1277.23	J/mol×K	1097.99	Joback Method
cpg	1289.68	J/mol×K	1134.13	Joback Method
cpg	1301.00	J/mol×K	1170.27	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=U321486&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume