Sarcosine, N-(4-trifluoromethylbenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C25H38F3NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-19-32-23(30)20-29(2)24(31)2

InchiKey: BGUQEPCCSNJPDF-UHFFFAOYSA-N

Formula: C25H38F3NO3

SMILES: CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 457.57

Physical Properties

Property code	Value	Unit	Source
gf	-571.25	kJ/mol	Joback Method
hf	-1221.20	kJ/mol	Joback Method
hfus	63.39	kJ/mol	Joback Method
hvap	88.38	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	7.022		Crippen Method
mcvol	363.650	ml/mol	McGowan Method
pc	912.18	kPa	Joback Method
rinpol	2943.00		NIST Webbook
rinpol	2943.00		NIST Webbook
tb	940.24	K	Joback Method
tc	1151.76	K	Joback Method
tf	569.20	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.82	J/mol×K	940.24	Joback Method
cpg	1233.34	J/mol×K	975.49	Joback Method
cpg	1249.63	J/mol×K	1010.75	Joback Method
cpg	1264.79	J/mol×K	1046.00	Joback Method
cpg	1278.91	J/mol×K	1081.26	Joback Method
cpg	1292.09	J/mol×K	1116.51	Joback Method
cpg	1304.40	J/mol×K	1151.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321514&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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