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

Inchi: InChI=1S/C24H36F3NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-31-21(29)18-28(2)24(30)1

InchiKey: HGXVTMYFGPWVQR-UHFFFAOYSA-N

Formula: C24H36F3NO3

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

Mol. weight [g/mol]: 443.54

Physical Properties

Property code	Value	Unit	Source
gf	-601.77	kJ/mol	Joback Method
hf	-1214.75	kJ/mol	Joback Method
hfus	67.44	kJ/mol	Joback Method
hvap	88.77	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.420		Crippen Method
mcvol	349.560	ml/mol	McGowan Method
pc	938.64	kPa	Joback Method
rinpol	2958.00		NIST Webbook
rinpol	2958.00		NIST Webbook
tb	930.55	K	Joback Method
tc	1140.26	K	Joback Method
tf	580.55	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.89	J/mol×K	930.55	Joback Method
cpg	1170.01	J/mol×K	965.50	Joback Method
cpg	1185.84	J/mol×K	1000.45	Joback Method
cpg	1200.44	J/mol×K	1035.41	Joback Method
cpg	1213.86	J/mol×K	1070.36	Joback Method
cpg	1226.14	J/mol×K	1105.31	Joback Method
cpg	1237.36	J/mol×K	1140.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321485&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

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