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

Inchi: InChI=1S/C22H32F3NO3/c1-3-4-5-6-7-8-9-10-11-16-29-20(27)17-26(2)21(28)18-12-14-1

InchiKey: FAIYOIMAQQRFNC-UHFFFAOYSA-N

Formula: C22H32F3NO3

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

Mol. weight [g/mol]: 415.49

Physical Properties

Property code	Value	Unit	Source
gf	-596.51	kJ/mol	Joback Method
hf	-1159.28	kJ/mol	Joback Method
hfus	55.62	kJ/mol	Joback Method
hvap	81.70	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.851		Crippen Method
mcvol	321.380	ml/mol	McGowan Method
pc	1094.27	kPa	Joback Method
rinpol	2588.00		NIST Webbook
rinpol	2588.00		NIST Webbook
tb	871.60	K	Joback Method
tc	1068.71	K	Joback Method
tf	535.39	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.56	J/mol×K	871.60	Joback Method
cpg	1048.76	J/mol×K	904.45	Joback Method
cpg	1063.88	J/mol×K	937.30	Joback Method
cpg	1078.00	J/mol×K	970.16	Joback Method
cpg	1091.18	J/mol×K	1003.01	Joback Method
cpg	1103.48	J/mol×K	1035.86	Joback Method
cpg	1114.97	J/mol×K	1068.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321512&Units=SI

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