Sarcosine, N-(2-trifluoromethylbenzoyl)-, dodecyl ester

Inchi: InChI=1S/C23H34F3NO3/c1-3-4-5-6-7-8-9-10-11-14-17-30-21(28)18-27(2)22(29)19-15-1

InchiKey: JSQFEUZPHYZXFV-UHFFFAOYSA-N

Formula: C23H34F3NO3

SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 429.52

Physical Properties

Property code	Value	Unit	Source
gf	-588.09	kJ/mol	Joback Method
hf	-1179.92	kJ/mol	Joback Method
hfus	58.21	kJ/mol	Joback Method
hvap	83.93	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	6.242		Crippen Method
mcvol	335.470	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	2756.00		NIST Webbook
rinpol	2756.00		NIST Webbook
tb	894.48	K	Joback Method
tc	1095.46	K	Joback Method
tf	546.66	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.02	J/mol×K	894.48	Joback Method
cpg	1109.61	J/mol×K	927.98	Joback Method
cpg	1125.08	J/mol×K	961.47	Joback Method
cpg	1139.52	J/mol×K	994.97	Joback Method
cpg	1152.98	J/mol×K	1028.46	Joback Method
cpg	1165.55	J/mol×K	1061.96	Joback Method
cpg	1177.29	J/mol×K	1095.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321330&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