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

Inchi: InChI=1S/C22H32F3NO3/c1-3-4-5-6-7-8-9-10-11-12-15-29-19(27)16-26(2)22(28)17-13-1

InchiKey: KGDYAPNFVWFSLP-UHFFFAOYSA-N

Formula: C22H32F3NO3

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

Mol. weight [g/mol]: 415.49

Physical Properties

Property code	Value	Unit	Source
gf	-618.61	kJ/mol	Joback Method
hf	-1173.47	kJ/mol	Joback Method
hfus	62.26	kJ/mol	Joback Method
hvap	84.32	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	5.640		Crippen Method
mcvol	321.380	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	2703.00		NIST Webbook
tb	884.79	K	Joback Method
tc	1083.39	K	Joback Method
tf	558.01	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.83	J/mol×K	884.79	Joback Method
cpg	1047.04	J/mol×K	917.89	Joback Method
cpg	1062.12	J/mol×K	950.99	Joback Method
cpg	1076.11	J/mol×K	984.09	Joback Method
cpg	1089.06	J/mol×K	1017.19	Joback Method
cpg	1101.00	J/mol×K	1050.29	Joback Method
cpg	1111.98	J/mol×K	1083.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321484&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