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

Inchi: InChI=1S/C21H30F3NO3/c1-3-4-5-6-7-8-9-10-11-14-28-18(26)15-25(2)21(27)16-12-13-1

InchiKey: HZYDPMLZRNECLO-UHFFFAOYSA-N

Formula: C21H30F3NO3

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

Mol. weight [g/mol]: 401.46

Physical Properties

Property code	Value	Unit	Source
gf	-627.03	kJ/mol	Joback Method
hf	-1152.83	kJ/mol	Joback Method
hfus	59.67	kJ/mol	Joback Method
hvap	82.10	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.250		Crippen Method
mcvol	307.290	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	861.91	K	Joback Method
tc	1056.37	K	Joback Method
tf	546.74	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.78	J/mol×K	861.91	Joback Method
cpg	986.56	J/mol×K	894.32	Joback Method
cpg	1001.29	J/mol×K	926.73	Joback Method
cpg	1015.00	J/mol×K	959.14	Joback Method
cpg	1027.71	J/mol×K	991.55	Joback Method
cpg	1039.48	J/mol×K	1023.96	Joback Method
cpg	1050.32	J/mol×K	1056.37	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=U321483&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