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

Inchi: InChI=1S/C20H28F3NO3/c1-3-4-5-6-7-8-9-10-13-27-17(25)14-24(2)20(26)15-11-12-16(2

InchiKey: IBEYTGIWRQBLOR-UHFFFAOYSA-N

Formula: C20H28F3NO3

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

Mol. weight [g/mol]: 387.44

Physical Properties

Property code	Value	Unit	Source
gf	-635.45	kJ/mol	Joback Method
hf	-1132.19	kJ/mol	Joback Method
hfus	57.08	kJ/mol	Joback Method
hvap	79.87	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.860		Crippen Method
mcvol	293.200	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	2497.00		NIST Webbook
rinpol	2497.00		NIST Webbook
tb	839.03	K	Joback Method
tc	1030.20	K	Joback Method
tf	535.47	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.44	J/mol×K	839.03	Joback Method
cpg	926.83	J/mol×K	870.89	Joback Method
cpg	941.22	J/mol×K	902.75	Joback Method
cpg	954.64	J/mol×K	934.61	Joback Method
cpg	967.13	J/mol×K	966.48	Joback Method
cpg	978.70	J/mol×K	998.34	Joback Method
cpg	989.40	J/mol×K	1030.20	Joback Method

Sources

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=U321482&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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