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

Inchi: InChI=1S/C18H24F3NO3/c1-3-4-5-6-7-8-11-25-15(23)12-22(2)18(24)13-9-10-14(19)17(2
InchiKey: IMNLZVLCBITGER-UHFFFAOYSA-N
Formula: C18H24F3NO3
SMILES: CCCCCCCCOC(=O)CN(C)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 359.38

Physical Properties

Property code	Value	Unit	Source
gf	-652.29	kJ/mol	Joback Method
hf	-1090.91	kJ/mol	Joback Method
hfus	51.90	kJ/mol	Joback Method
hvap	75.42	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.080		Crippen Method
mcvol	265.020	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
tb	793.27	K	Joback Method
tc	980.16	K	Joback Method
tf	512.93	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.21	J/mol×K	793.27	Joback Method
cpg	809.83	J/mol×K	824.42	Joback Method
cpg	823.55	J/mol×K	855.57	Joback Method
cpg	836.40	J/mol×K	886.72	Joback Method
cpg	848.39	J/mol×K	917.87	Joback Method
cpg	859.55	J/mol×K	949.01	Joback Method
cpg	869.91	J/mol×K	980.16	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=U321480&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