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

Inchi: InChI=1S/C15H18F3NO3/c1-3-4-5-8-22-12(20)9-19(2)15(21)10-6-7-11(16)14(18)13(10)1

InchiKey: FLDLLMWWRFPUAD-UHFFFAOYSA-N

Formula: C15H18F3NO3

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

Mol. weight [g/mol]: 317.30

Physical Properties

Property code	Value	Unit	Source
gf	-677.55	kJ/mol	Joback Method
hf	-1028.99	kJ/mol	Joback Method
hfus	44.13	kJ/mol	Joback Method
hvap	68.74	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	2.909		Crippen Method
mcvol	222.750	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	1996.00		NIST Webbook
rinpol	1996.00		NIST Webbook
tb	724.63	K	Joback Method
tc	910.00	K	Joback Method
tf	479.12	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.00	J/mol×K	724.63	Joback Method
cpg	641.41	J/mol×K	755.52	Joback Method
cpg	654.04	J/mol×K	786.42	Joback Method
cpg	665.90	J/mol×K	817.31	Joback Method
cpg	677.01	J/mol×K	848.21	Joback Method
cpg	687.39	J/mol×K	879.10	Joback Method
cpg	697.06	J/mol×K	910.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321477&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