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

Inchi: InChI=1S/C17H22F3NO3/c1-3-4-5-6-7-10-24-14(22)11-21(2)17(23)12-8-9-13(18)16(20)1

InchiKey: LWLPJUOBCRLQGF-UHFFFAOYSA-N

Formula: C17H22F3NO3

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

Mol. weight [g/mol]: 345.36

Physical Properties

Property code	Value	Unit	Source
gf	-660.71	kJ/mol	Joback Method
hf	-1070.27	kJ/mol	Joback Method
hfus	49.31	kJ/mol	Joback Method
hvap	73.19	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.690		Crippen Method
mcvol	250.930	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
rinpol	2186.00		NIST Webbook
rinpol	2186.00		NIST Webbook
tb	770.39	K	Joback Method
tc	956.18	K	Joback Method
tf	501.66	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.45	J/mol×K	770.39	Joback Method
cpg	752.69	J/mol×K	801.35	Joback Method
cpg	766.06	J/mol×K	832.32	Joback Method
cpg	778.60	J/mol×K	863.28	Joback Method
cpg	790.32	J/mol×K	894.25	Joback Method
cpg	801.25	J/mol×K	925.21	Joback Method
cpg	811.41	J/mol×K	956.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321479&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

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