Sarcosine, N-(2-trifluoromethylbenzoyl)-, heptadecyl ester

Inchi: InChI=1S/C28H44F3NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-35-26(33)23-32(

InchiKey: PBQJSQSEIVZRBI-UHFFFAOYSA-N

Formula: C28H44F3NO3

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 499.65

Physical Properties

Property code	Value	Unit	Source
gf	-545.99	kJ/mol	Joback Method
hf	-1283.12	kJ/mol	Joback Method
hfus	71.16	kJ/mol	Joback Method
hvap	95.06	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.192		Crippen Method
mcvol	405.920	ml/mol	McGowan Method
pc	772.03	kPa	Joback Method
tb	1008.88	K	Joback Method
tc	1244.45	K	Joback Method
tf	603.01	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1404.15	J/mol×K	1008.88	Joback Method
cpg	1423.49	J/mol×K	1048.14	Joback Method
cpg	1441.39	J/mol×K	1087.40	Joback Method
cpg	1457.98	J/mol×K	1126.66	Joback Method
cpg	1473.41	J/mol×K	1165.92	Joback Method
cpg	1487.81	J/mol×K	1205.18	Joback Method
cpg	1501.32	J/mol×K	1244.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321334&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume