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

Inchi: InChI=1S/C17H22F3NO3/c1-3-4-5-8-11-24-15(22)12-21(2)16(23)13-9-6-7-10-14(13)17(1

InchiKey: DTKZQPOJZYYLDL-UHFFFAOYSA-N

Formula: C17H22F3NO3

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

Mol. weight [g/mol]: 345.36

Physical Properties

Property code	Value	Unit	Source
gf	-638.61	kJ/mol	Joback Method
hf	-1056.08	kJ/mol	Joback Method
hfus	42.67	kJ/mol	Joback Method
hvap	70.57	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.901		Crippen Method
mcvol	250.930	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	2136.00		NIST Webbook
tb	757.20	K	Joback Method
tc	946.55	K	Joback Method
tf	479.04	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.87	J/mol×K	757.20	Joback Method
cpg	756.44	J/mol×K	788.76	Joback Method
cpg	770.07	J/mol×K	820.32	Joback Method
cpg	782.80	J/mol×K	851.87	Joback Method
cpg	794.70	J/mol×K	883.43	Joback Method
cpg	805.79	J/mol×K	914.99	Joback Method
cpg	816.13	J/mol×K	946.55	Joback Method

Sources

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=U321324&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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