Sarcosine, N-(4-trifluoromethylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C18H24F3NO3/c1-3-4-5-6-7-12-25-16(23)13-22(2)17(24)14-8-10-15(11-9-14)1

InchiKey: JQJWZMZOGUYDAZ-UHFFFAOYSA-N

Formula: C18H24F3NO3

SMILES: CCCCCCCOC(=O)CN(C)C(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 359.38

Physical Properties

Property code	Value	Unit	Source
gf	-630.19	kJ/mol	Joback Method
hf	-1076.72	kJ/mol	Joback Method
hfus	45.26	kJ/mol	Joback Method
hvap	72.80	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.291		Crippen Method
mcvol	265.020	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	2188.00		NIST Webbook
tb	780.08	K	Joback Method
tc	969.64	K	Joback Method
tf	490.31	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.27	J/mol×K	780.08	Joback Method
cpg	813.15	J/mol×K	811.67	Joback Method
cpg	827.07	J/mol×K	843.27	Joback Method
cpg	840.08	J/mol×K	874.86	Joback Method
cpg	852.23	J/mol×K	906.45	Joback Method
cpg	863.57	J/mol×K	938.04	Joback Method
cpg	874.15	J/mol×K	969.64	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=U321508&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