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

Inchi: InChI=1S/C16H20F3NO3/c1-3-4-5-10-23-14(21)11-20(2)15(22)12-6-8-13(9-7-12)16(17,1

InchiKey: FRMWCESCCWPBDZ-UHFFFAOYSA-N

Formula: C16H20F3NO3

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

Mol. weight [g/mol]: 331.33

Physical Properties

Property code	Value	Unit	Source
gf	-647.03	kJ/mol	Joback Method
hf	-1035.44	kJ/mol	Joback Method
hfus	40.08	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.511		Crippen Method
mcvol	236.840	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2000.00		NIST Webbook
tb	734.32	K	Joback Method
tc	924.03	K	Joback Method
tf	467.77	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.47	J/mol×K	734.32	Joback Method
cpg	700.71	J/mol×K	765.94	Joback Method
cpg	714.04	J/mol×K	797.56	Joback Method
cpg	726.48	J/mol×K	829.17	Joback Method
cpg	738.10	J/mol×K	860.79	Joback Method
cpg	748.93	J/mol×K	892.41	Joback Method
cpg	759.01	J/mol×K	924.03	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=U321506&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