1-Propanone, 1-[3,5-bis(trifluoromethyl)phenyl]-

Other names: 3',5'-Bis(trifluoromethyl)propiophenone
Inchi: InChI=1S/C11H8F6O/c1-2-9(18)6-3-7(10(12,13)14)5-8(4-6)11(15,16)17/h3-5H,2H2,1H3
InchiKey: VLRWCHKOSBUGMB-UHFFFAOYSA-N
Formula: C11H8F6O
SMILES: CCC(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 270.17
CAS: 85068-34-4

Physical Properties

Property code	Value	Unit	Source
gf	-1157.21	kJ/mol	Joback Method
hf	-1363.52	kJ/mol	Joback Method
hfus	22.76	kJ/mol	Joback Method
hvap	42.93	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.317		Crippen Method
mcvol	154.280	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
tb	530.75	K	Joback Method
tc	710.40	K	Joback Method
tf	323.50	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.73	J/mol×K	530.75	Joback Method
cpg	389.83	J/mol×K	560.69	Joback Method
cpg	401.13	J/mol×K	590.63	Joback Method
cpg	411.65	J/mol×K	620.58	Joback Method
cpg	421.45	J/mol×K	650.52	Joback Method
cpg	430.57	J/mol×K	680.46	Joback Method
cpg	439.05	J/mol×K	710.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85068344&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