3,5-bis(trifluoromethyl)benzophenone

Inchi: InChI=1S/C15H8F6O/c16-14(17,18)11-6-10(7-12(8-11)15(19,20)21)13(22)9-4-2-1-3-5-9/
InchiKey: QETSMUIBVUASOJ-UHFFFAOYSA-N
Formula: C15H8F6O
SMILES: O=C(c1ccccc1)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 318.21
CAS: 21221-93-2

Physical Properties

Property code	Value	Unit	Source
gf	-1011.12	kJ/mol	Joback Method
hf	-1209.55	kJ/mol	Joback Method
hfus	27.16	kJ/mol	Joback Method
hvap	54.11	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.955		Crippen Method
mcvol	186.880	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
tb	648.95	K	Joback Method
tc	855.70	K	Joback Method
tf	395.00	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.00	J/mol×K	648.95	Joback Method
cpg	506.78	J/mol×K	683.41	Joback Method
cpg	518.49	J/mol×K	717.87	Joback Method
cpg	529.21	J/mol×K	752.32	Joback Method
cpg	539.01	J/mol×K	786.78	Joback Method
cpg	547.99	J/mol×K	821.24	Joback Method
cpg	556.22	J/mol×K	855.70	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=C21221932&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume