3,3',5,5'-Tetrakis(trifluoromethyl)benzophenone

Inchi: InChI=1S/C17H6F12O/c18-14(19,20)9-1-7(2-10(5-9)15(21,22)23)13(30)8-3-11(16(24,25)
InchiKey: GATWMPGNBWPCIY-UHFFFAOYSA-N
Formula: C17H6F12O
SMILES: O=C(c1cc(C(F)(F)F)cc(C(F)(F)F)c1)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 454.21
CAS: 175136-66-0

Physical Properties

Property code	Value	Unit	Source
gf	-2176.72	kJ/mol	Joback Method
hf	-2467.93	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	52.39	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	6.993		Crippen Method
mcvol	225.680	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
tb	693.83	K	Joback Method
tc	873.34	K	Joback Method
tf	450.96	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.73	J/mol×K	693.83	Joback Method
cpg	658.61	J/mol×K	723.75	Joback Method
cpg	668.59	J/mol×K	753.67	Joback Method
cpg	677.75	J/mol×K	783.58	Joback Method
cpg	686.18	J/mol×K	813.50	Joback Method
cpg	693.95	J/mol×K	843.42	Joback Method
cpg	701.13	J/mol×K	873.34	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=C175136660&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