3,4'-Bis(trifluoromethyl)benzophenone

Other names: Benzophenone, 3,4'-bis(trifluoromethyl)-
3,4'-Bis(trifluoromethyl)benzophenone
Inchi: InChI=1S/C15H8F6O/c16-14(17,18)11-6-4-9(5-7-11)13(22)10-2-1-3-12(8-10)15(19,20)21
InchiKey: HWBXNAPXNCBCQO-UHFFFAOYSA-N
Formula: C15H8F6O
SMILES: O=C(c1ccc(C(F)(F)F)cc1)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 318.22

Physical Properties

Property code	Value	Unit	Source
hf	-1257.91	kJ/mol	Cheméo Relay (1.0)
hfus	27.16	kJ/mol	Joback Method
hvap	90.16	kJ/mol	Cheméo Relay (1.0)
ie	9.80	eV	Cheméo Relay (1.0)
log10ws	-5.68		Cheméo Relay (1.0)
logp	4.955		Crippen Method
mcvol	186.880	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
tb	573.34	K	Cheméo Relay (1.0)
tc	817.89	K	Cheméo Relay (1.0)
tf	381.74	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21084220&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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