Benzene, 1,2-bis(trifluoromethyl)-

Other names: o-Xylene, «alpha»,«alpha»,«alpha»,«alpha»',«alpha»',«alpha»'-hexafluoro-
1,2-Bis(trifluoromethyl)benzene
o-Bis(trifluoromethyl)benzene
Inchi: InChI=1S/C8H4F6/c9-7(10,11)5-3-1-2-4-6(5)8(12,13)14/h1-4H
InchiKey: XXZOEDQFGXTEAD-UHFFFAOYSA-N
Formula: C8H4F6
SMILES: FC(F)(F)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 214.11
CAS: 433-95-4

Physical Properties

Property code	Value	Unit	Source
gf	-1043.92	kJ/mol	Joback Method
hf	-1177.55	kJ/mol	Joback Method
hfus	13.78	kJ/mol	Joback Method
hvap	28.85	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.724		Crippen Method
mcvol	110.440	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	403.26	K	Joback Method
tc	575.71	K	Joback Method
tf	227.24	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.05	J/mol×K	403.26	Joback Method
cpg	241.61	J/mol×K	432.00	Joback Method
cpg	252.37	J/mol×K	460.74	Joback Method
cpg	262.39	J/mol×K	489.48	Joback Method
cpg	271.69	J/mol×K	518.23	Joback Method
cpg	280.31	J/mol×K	546.97	Joback Method

cpg	288.29	J/mol×K	575.71	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C433954&Units=SI

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