Benzene, hexakis(trifluoromethyl)-

Other names: Hexa[trifluoromethyl]benzene
Inchi: InChI=1S/C12F18/c13-7(14,15)1-2(8(16,17)18)4(10(22,23)24)6(12(28,29)30)5(11(25,26)
InchiKey: XJGMLRCIWIZTKI-UHFFFAOYSA-N
Formula: C12F18
SMILES: FC(F)(F)c1c(C(F)(F)F)c(C(F)(F)F)c(C(F)(F)F)c(C(F)(F)F)c(C(F)(F)F)c1C(F)(F)F
Mol. weight [g/mol]: 486.10
CAS: 2340-93-4

Physical Properties

Property code	Value	Unit	Source
gf	-3375.12	kJ/mol	Joback Method
hf	-3694.31	kJ/mol	Joback Method
hfus	29.89	kJ/mol	Joback Method
hvap	25.41	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.799		Crippen Method
mcvol	188.040	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
tb	493.02	K	Joback Method
tc	622.30	K	Joback Method
tf	339.16	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.94	J/mol×K	493.02	Joback Method
cpg	524.74	J/mol×K	514.57	Joback Method
cpg	534.82	J/mol×K	536.11	Joback Method
cpg	544.20	J/mol×K	557.66	Joback Method
cpg	552.93	J/mol×K	579.21	Joback Method
cpg	561.04	J/mol×K	600.76	Joback Method
cpg	568.56	J/mol×K	622.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2340934&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