

Benzene, 1,4-bis(trifluoromethyl)-

Other names:	1,4-Bis(trifluoromethyl)benzene 1,4-di(Trifluoromethyl)benzene Hexafluoro-p-xylene NSC 61992 alpha,alpha,alpha,alpha',alpha',alpha'-Hexafluoro-p-xylene p-Bis(trifluoromethyl)benzene p-Trifluoromethylbenzotrifluoride p-Xylene, alpha,alpha,alpha,alpha',alpha',alpha'-hexafluoro- p-Xylene, «alpha»,«alpha»,«alpha»,«alpha'»,«alpha'»,«alpha'»-hexafluoro- p-Xylene, Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ'»,Â«alphaÂ'»,Â«alphaÂ'»-hexafluoro- «alpha»,«alpha»,«alpha»,«alpha»,«alpha»,«alpha»-Hexafluoro-p-xylene Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ'»,Â«alphaÂ'»,Â«alphaÂ'»-Hexafluoro-p-xylene
Inchi:	InChI=1S/C8H4F6/c9-7(10,11)5-1-2-6(4-3-5)8(12,13)14/h1-4H
InchiKey:	PDCBZHHORLHNCZ-UHFFFAOYSA-N
Formula:	C8H4F6
SMILES:	FC(F)(F)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	214.11
CAS:	433-19-2

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
ie	10.43 ± 0.05	eV	NIST Webbook
log10ws	-3.68		Crippen Method
logp	3.724		Crippen Method
mcvol	110.440	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	389.20	K	NIST Webbook
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
hvapt	41.80	kJ/mol	338.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.09616e+01
Coeff. B	-2.38439e+03
Coeff. C	-6.46190e+01
Temperature range (K), min.	288.00
Temperature range (K), max.	486.62

Sources

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=C433192&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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