Benzene, 1,3-bis(trifluoromethyl)-

Other names:	1,3-Bis(trifluoromethyl)benzene 1,3-di(Trifluoromethyl)benzene NSC 10342 m-Bis(trifluoromethyl)benzene m-Xylene, «alpha»,«alpha»,«alpha»,«alpha»',«alpha»',«alpha»'-hexafluoro- m-Xylene, Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»',Â«alphaÂ»',Â«alphaÂ»'-hexafluoro- «alpha»,«alpha»,«alpha»,«alpha»',«alpha»',«alpha»'-Hexafluoro-m-xylene «alpha»,«alpha»,«alpha»,«beta»,«beta»,«beta»-hexafluoro-m-xylene «alpha»«alpha»«alpha»-«alpha»',«alpha»',«alpha»' -Hexafluoro-m-xylol Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»',Â«alphaÂ»',Â«alphaÂ»'-Hexafluoro-m-xyl Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»,Â«betaÂ»,Â«betaÂ»,Â«betaÂ»-hexafluoro-m-xylene Â«alphaÂ»Â«alphaÂ»Â«alphaÂ»-Â«alphaÂ»',Â«alphaÂ»',Â«alphaÂ»' -Hexafluoro-m-xylol
Inchi:	InChI=1S/C8H4F6/c9-7(10,11)5-2-1-3-6(4-5)8(12,13)14/h1-4H
InchiKey:	SJBBXFLOLUTGCW-UHFFFAOYSA-N
Formula:	C8H4F6
SMILES:	FC(F)(F)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	214.11
CAS:	402-31-3

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	10.57	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
rinpol	700.00		NIST Webbook
tb	389.00	K	NIST Webbook
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	42.40	kJ/mol	314.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.13385e+01
Coeff. B	-2.60627e+03
Coeff. C	-5.26790e+01
Temperature range (K), min.	275.00
Temperature range (K), max.	485.11

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=C402313&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume