

Benzene, 2,4-dichloro-1-(trifluoromethyl)-

Other names:	1,3-DICHLORO-4-(TRIFLUOROMETYL)BENZENE 1,3-Dichloro-4-(trifluoromethyl)benzene 2,4-Dichloro-1-(trifluoromethyl)benzene 2,4-Dichlorobenzotrifluoride 2,4-dichloro-«alpha», «alpha», «alpha»-trifluorotoluene 2,4-dichloro-Â«alphaÂ», Â«alphaÂ», Â«alphaÂ»-trifluorotoluene
Inchi:	InChI=1S/C7H3Cl2F3/c8-4-1-2-5(6(9)3-4)7(10,11)12/h1-3H
InchiKey:	KALSHRGEFLVFHE-UHFFFAOYSA-N
Formula:	C7H3Cl2F3
SMILES:	FC(F)(F)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	215.00
CAS:	320-60-5

Physical Properties

Property code	Value	Unit	Source
gf	-504.24	kJ/mol	Joback Method
hf	-602.78	kJ/mol	Joback Method
hfus	17.37	kJ/mol	Joback Method
hvap	39.80	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	4.012		Crippen Method
mcvol	115.520	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	390.70	K	NIST Webbook
tb	390.50 ± 0.50	K	NIST Webbook
tc	673.39	K	Joback Method
tf	284.14	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.20	J/molxK	465.64	Joback Method
cpg	224.05	J/molxK	500.26	Joback Method

cpg	232.21	J/mol×K	534.89	Joback Method
cpg	239.74	J/mol×K	569.51	Joback Method
cpg	246.66	J/mol×K	604.14	Joback Method
cpg	253.01	J/mol×K	638.76	Joback Method
cpg	258.84	J/mol×K	673.39	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45538e+01
Coeff. B	-3.86291e+03
Coeff. C	-6.18510e+01
Temperature range (K), min.	332.62
Temperature range (K), max.	479.81

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.04011e+01
Coeff. B	-8.73865e+03
Coeff. C	-9.36249e+00
Coeff. D	3.91306e-06
Temperature range (K), min.	247.55
Temperature range (K), max.	646.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C320605&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1688
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1688.mol

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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