1,2,3,5-TETRAFLUOROBENZENE

Other names: 1,2,4,6-tetrafluorobenzene
1,3,4,5-tetrafluorobenzene
benzene, 1,2,3,5-tetrafluoro-
Inchi: InChI=1S/C6H2F4/c7-3-1-4(8)6(10)5(9)2-3/h1-2H
InchiKey: UHHYOKRQTQBKSB-UHFFFAOYSA-N
Formula: C6H2F4
SMILES: Fc1cc(F)c(F)c(F)c1
Mol. weight [g/mol]: 150.07
CAS: 2367-82-0

Physical Properties

Property code	Value	Unit	Source
af	0.3460		KDB
hf	-628.26	kJ/mol	Cheméo Relay (1.0)
hfus	16.49	kJ/mol	Joback Method
hvap	36.22	kJ/mol	Cheméo Relay (1.0)
ie	9.53	eV	Cheméo Relay (1.0)
log10ws	-2.31		Aqueous Solubility Prediction Method
logp	2.243		Crippen Method
mcvol	78.720	ml/mol	McGowan Method
pc	3747.00	kPa	KDB
tb	357.61	K	KDB
tc	535.25	K	KDB
tf	225.00	K	KDB
vc	0.313	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.11	J/mol×K	375.38	Joback Method
cpg	147.59	J/mol×K	404.29	Joback Method
cpg	153.81	J/mol×K	433.20	Joback Method
cpg	159.77	J/mol×K	462.11	Joback Method

cpg	165.47	J/mol×K	491.02	Joback Method
cpg	170.93	J/mol×K	519.93	Joback Method
cpg	176.14	J/mol×K	548.84	Joback Method
rhol	1403.00	kg/m3	296.30	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide
rhol	1352.00	kg/m3	325.90	Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66435e+01
Coeff. B	-3.46280e+03
Coeff. C	-5.13750e+01
Temperature range (K), min.	263.09
Temperature range (K), max.	356.95

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.97998e+01
Coeff. B	-6.81695e+03
Coeff. C	-9.70897e+00
Coeff. D	7.53476e-06
Temperature range (K), min.	279.15
Temperature range (K), max.	535.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1668
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2367820&Units=SI
Liquid-Liquid Equilibria in Binary Mixtures Containing Fluorinated Benzenes and Ionic Liquid	https://www.doi.org/10.1021/je8006474
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Cheméo Relay (1.0, beta):	
1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide:	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1668.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume