2,5-Dichlorobenzotrifluoride

Other names: Benzene, 1,4-dichloro-2-(trifluoromethyl)-
2,5-Dichloro-«alpha»,«alpha»,«alpha»-trifluorotoluene
1,4-dichloro-2-(trifluoromethyl)benzene
Inchi: InChI=1S/C7H3Cl2F3/c8-4-1-2-6(9)5(3-4)7(10,11)12/h1-3H
InchiKey: DYBYUWVMLBBEMA-UHFFFAOYSA-N
Formula: C7H3Cl2F3
SMILES: FC(F)(F)c1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 215.00
CAS: 320-50-3

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
rinpol	1007.00		NIST Webbook
rinpol	1007.00		NIST Webbook
tb	465.64	K	Joback Method
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/mol×K	465.64	Joback Method
cpg	224.05	J/mol×K	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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C320503&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume