Benzene, 1-dichloromethyl-3-fluoro

Other names: 1-(dichloromethyl)-3-fluorobenzene
Inchi: InChI=1S/C7H5Cl2F/c8-7(9)5-2-1-3-6(10)4-5/h1-4,7H
InchiKey: MVRCPAOYPLZMLB-UHFFFAOYSA-N
Formula: C7H5Cl2F
SMILES: Fc1cccc(C(Cl)Cl)c1
Mol. weight [g/mol]: 179.02
CAS: 402-64-2

Physical Properties

Property code	Value	Unit	Source
gf	-110.27	kJ/mol	Joback Method
hf	-195.62	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	41.68	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.302		Crippen Method
mcvol	111.980	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
tb	464.91	K	Joback Method
tc	685.73	K	Joback Method
tf	253.02	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.41	J/mol×K	464.91	Joback Method
cpg	204.98	J/mol×K	501.71	Joback Method
cpg	213.90	J/mol×K	538.52	Joback Method
cpg	222.22	J/mol×K	575.32	Joback Method
cpg	229.94	J/mol×K	612.13	Joback Method
cpg	237.11	J/mol×K	648.93	Joback Method

cpg	243.76	J/mol×K	685.73	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C402642&Units=SI

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