

Benzyl alcohol, p-fluoro-alpha-(trichloromethyl)-

Inchi:	InChI=1S/C8H6Cl3FO/c9-8(10,11)7(13)5-1-3-6(12)4-2-5/h1-4,7,13H
InchiKey:	NXMVOAIYDICRQK-UHFFFAOYSA-N
Formula:	C8H6Cl3FO
SMILES:	OC(c1ccc(F)cc1)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	243.49
CAS:	394-56-9

Physical Properties

Property code	Value	Unit	Source
gf	-247.76	kJ/mol	Joback Method
hf	-392.98	kJ/mol	Joback Method
hfus	18.95	kJ/mol	Joback Method
hvap	63.67	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.229		Crippen Method
mcvol	144.180	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	614.17	K	Joback Method
tc	832.57	K	Joback Method
tf	357.45	K	Joback Method
vc	0.542	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.11	J/mol×K	614.17	Joback Method
cpg	311.42	J/mol×K	650.57	Joback Method
cpg	319.02	J/mol×K	686.97	Joback Method
cpg	325.96	J/mol×K	723.37	Joback Method
cpg	332.29	J/mol×K	759.77	Joback Method
cpg	338.07	J/mol×K	796.17	Joback Method
cpg	343.37	J/mol×K	832.57	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=C394569&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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