Benzene, (2,2-dichloro-1,1,2-trifluoroethyl)-3-(fluorosulfonyl

Inchi: InChI=1S/C8H4Cl2F4O2S/c9-8(10,13)7(11,12)5-2-1-3-6(4-5)17(14,15)16/h1-4H

InchiKey: XUSPAHZOHZRAPT-UHFFFAOYSA-N

Formula: C8H4Cl2F4O2S

SMILES: O=S(=O)(F)c1cccc(C(F)(F)C(F)(Cl)Cl)c1

Mol. weight [g/mol]: 311.08

Physical Properties

Property code	Value	Unit	Source
gf	-1146.70	kJ/mol	Joback Method
hf	-1270.16	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	57.89	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.538		Crippen Method
mcvol	159.470	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1386.00		NIST Webbook
tb	527.36	K	Joback Method
tc	726.67	K	Joback Method
tf	324.46	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.52	J/mol×K	527.36	Joback Method
cpg	352.39	J/mol×K	560.58	Joback Method
cpg	362.35	J/mol×K	593.80	Joback Method
cpg	371.43	J/mol×K	627.01	Joback Method
cpg	379.69	J/mol×K	660.23	Joback Method
cpg	387.18	J/mol×K	693.45	Joback Method
cpg	393.93	J/mol×K	726.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R504246&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