Benzene, 1-fluoro-3-trichloromethyl

Other names: m-fluoro-«alpha»,«alpha»,«alpha»-trichlorotoluene
Inchi: InChI=1S/C7H4Cl3F/c8-7(9,10)5-2-1-3-6(11)4-5/h1-4H
InchiKey: JRTYPYSADXRJBQ-UHFFFAOYSA-N
Formula: C7H4Cl3F
SMILES: Fc1cccc(C(Cl)(Cl)Cl)c1
Mol. weight [g/mol]: 213.46
CAS: 401-77-4

Physical Properties

Property code	Value	Unit	Source
gf	-116.92	kJ/mol	Joback Method
hf	-214.83	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	45.16	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.652		Crippen Method
mcvol	124.220	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	1168.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1168.00		NIST Webbook
tb	499.55	K	Joback Method
tc	736.18	K	Joback Method
tf	300.36	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.81	J/mol×K	499.55	Joback Method
cpg	230.24	J/mol×K	538.99	Joback Method
cpg	238.80	J/mol×K	578.43	Joback Method
cpg	246.53	J/mol×K	617.86	Joback Method
cpg	253.51	J/mol×K	657.30	Joback Method

cpg	259.80	J/mol×K	696.74	Joback Method
cpg	265.47	J/mol×K	736.18	Joback Method

Sources

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=C401774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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