2,3-Dichloro-1,1,1-trifluoro-2-methylpropane

Inchi: InChI=1S/C4H5Cl2F3/c1-3(6,2-5)4(7,8)9/h2H2,1H3
InchiKey: IPJDLVJQVSOCBI-UHFFFAOYSA-N
Formula: C4H5Cl2F3
SMILES: CC(Cl)(CCl)C(F)(F)F
Mol. weight [g/mol]: 180.98
CAS: 374-18-5

Physical Properties

Property code	Value	Unit	Source
gf	-619.81	kJ/mol	Joback Method
hf	-763.20	kJ/mol	Joback Method
hfus	8.92	kJ/mol	Joback Method
hvap	28.23	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.785		Crippen Method
mcvol	97.010	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	366.50 ± 0.50	K	NIST Webbook
tc	532.21	K	Joback Method
tf	201.29	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.56	J/mol×K	357.13	Joback Method
cpg	177.52	J/mol×K	386.31	Joback Method
cpg	185.84	J/mol×K	415.49	Joback Method
cpg	193.55	J/mol×K	444.67	Joback Method
cpg	200.68	J/mol×K	473.85	Joback Method
cpg	207.25	J/mol×K	503.03	Joback Method
cpg	213.32	J/mol×K	532.21	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=C374185&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume