1,1,1-Trichloro-3,3,3-trifluoropropane

Inchi: InChI=1S/C3H2Cl3F3/c4-2(5,6)1-3(7,8)9/h1H2
InchiKey: MDNLZVVUMKSEKO-UHFFFAOYSA-N
Formula: C3H2Cl3F3
SMILES: FC(F)(F)CC(Cl)(Cl)Cl
Mol. weight [g/mol]: 201.40
CAS: 7125-84-0

Physical Properties

Property code	Value	Unit	Source
chl	-1234.30 ± 0.92	kJ/mol	NIST Webbook
gf	-640.16	kJ/mol	Joback Method
hf	-758.30	kJ/mol	Joback Method
hfl	-830.65 ± 0.92	kJ/mol	NIST Webbook
hfus	10.53	kJ/mol	Joback Method
hvap	36.80 ± 0.10	kJ/mol	NIST Webbook
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	95.160	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	371.68	K	Joback Method
tc	556.18	K	Joback Method
tf	219.94	K	Joback Method
tt	232.69 ± 0.02	K	NIST Webbook
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.55	J/mol×K	494.68	Joback Method
cpg	188.37	J/mol×K	525.43	Joback Method
cpg	158.67	J/mol×K	371.68	Joback Method
cpg	165.81	J/mol×K	402.43	Joback Method
cpg	172.31	J/mol×K	433.18	Joback Method
cpg	178.22	J/mol×K	463.93	Joback Method

cpg	192.69	J/mol×K	556.18	Joback Method
hfust	14.07	kJ/mol	232.70	NIST Webbook
hvapt	35.20	kJ/mol	342.50	NIST Webbook

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=C7125840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tt:	Triple Point Temperature
vc:	Critical Volume

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