

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:

7125-83-9

Physical Properties

Property code	Value	Unit	Source
gf	-640.16	kJ/mol	Joback Method
hf	-758.30	kJ/mol	Joback Method
hfus	10.53	kJ/mol	Joback Method
hvap	30.38	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	95.160	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
sl	311.42	J/mol×K	NIST Webbook
tb	371.68	K	Joback Method
tc	556.18	K	Joback Method
tf	219.94	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.22	J/mol×K	463.93	Joback Method
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	192.69	J/mol×K	556.18	Joback Method
cpl	199.91	J/mol×K	298.15	NIST Webbook

hfust	14.07	kJ/mol	232.69	NIST Webbook
sfust	60.45	J/mol×K	232.69	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=C7125839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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