1-Chloro-3,3,3-trifluoro-2-methylpropene

Inchi: InChI=1S/C4H4ClF3/c1-3(2-5)4(6,7)8/h1-2H2
InchiKey: DHODLDAVSMRUMX-UHFFFAOYSA-N
Formula: C4H4ClF3
SMILES: C=C(CCl)C(F)(F)F
Mol. weight [g/mol]: 144.52
CAS: 381-83-9

Physical Properties

Property code	Value	Unit	Source
gf	-531.43	kJ/mol	Joback Method
hf	-623.07	kJ/mol	Joback Method
hfus	9.55	kJ/mol	Joback Method
hvap	24.55	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.344		Crippen Method
mcvol	80.470	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	319.00	K	NIST Webbook
tb	319.60 ± 2.00	K	NIST Webbook
tc	480.70	K	Joback Method
tf	152.90 ± 3.00	K	NIST Webbook
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.14	J/mol×K	319.49	Joback Method
cpg	138.56	J/mol×K	346.36	Joback Method
cpg	145.54	J/mol×K	373.23	Joback Method
cpg	152.11	J/mol×K	400.10	Joback Method
cpg	158.28	J/mol×K	426.97	Joback Method
cpg	164.07	J/mol×K	453.84	Joback Method
cpg	169.49	J/mol×K	480.70	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=C381839&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

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