Trifluoromethylcyclohexane

Other names: CYCLO-HEXYLFLUOROFORM
Inchi: InChI=1S/C7H11F3/c8-7(9,10)6-4-2-1-3-5-6/h6H,1-5H2
InchiKey: QXPZOKVSFMRGMQ-UHFFFAOYSA-N
Formula: C7H11F3
SMILES: FC(F)(F)C1CCCCC1
Mol. weight [g/mol]: 152.16
CAS: 401-75-2

Physical Properties

Property code	Value	Unit	Source
gf	-549.08	kJ/mol	Joback Method
hf	-730.57	kJ/mol	Joback Method
hfus	7.55	kJ/mol	Joback Method
hvap	27.86	kJ/mol	Joback Method
ie	10.46 ± 0.02	eV	NIST Webbook
log10ws	-3.07		Crippen Method
logp	3.129		Crippen Method
mcvol	103.940	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
tb	380.35	K	KDB
tc	555.94	K	Joback Method
tf	180.22	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.38	J/mol×K	373.69	Joback Method
cpg	213.08	J/mol×K	404.06	Joback Method
cpg	227.94	J/mol×K	434.44	Joback Method
cpg	242.00	J/mol×K	464.81	Joback Method
cpg	255.29	J/mol×K	495.19	Joback Method
cpg	267.82	J/mol×K	525.56	Joback Method
cpg	279.63	J/mol×K	555.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C401752&Units=SI
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1761.mol

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
ie:	Ionization energy
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