1-Chloro-2,3,3-trifluorocyclobutene

Inchi: InChI=1S/C4H2ClF3/c5-2-1-4(7,8)3(2)6/h1H2
InchiKey: NTBUBNMKBVNZBB-UHFFFAOYSA-N
Formula: C4H2ClF3
SMILES: FC1=C(Cl)CC1(F)F
Mol. weight [g/mol]: 142.51
CAS: 694-62-2

Physical Properties

Property code	Value	Unit	Source
gf	-559.70	kJ/mol	Joback Method
hf	-613.24	kJ/mol	Joback Method
hfus	9.73	kJ/mol	Joback Method
hvap	26.98	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.445		Crippen Method
mcvol	69.610	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	346.53	K	Joback Method
tc	524.99	K	Joback Method
tf	230.65	K	Joback Method
vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.69	J/mol×K	346.53	Joback Method
cpg	122.82	J/mol×K	376.27	Joback Method
cpg	129.27	J/mol×K	406.02	Joback Method
cpg	135.08	J/mol×K	435.76	Joback Method
cpg	140.33	J/mol×K	465.50	Joback Method
cpg	145.08	J/mol×K	495.25	Joback Method
cpg	149.37	J/mol×K	524.99	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=C694622&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