Acetonitrile, chlorodifluoro-

Other names: Chlorodifluoroacetonitrile
Inchi: InChI=1S/C2ClF2N/c3-2(4,5)1-6
InchiKey: GUIPZCNIFDPABQ-UHFFFAOYSA-N
Formula: C2ClF2N
SMILES: N#CC(F)(F)Cl
Mol. weight [g/mol]: 111.48
CAS: 421-05-6

Physical Properties

Property code	Value	Unit	Source
gf	-299.57	kJ/mol	Joback Method
hf	-336.44	kJ/mol	Joback Method
hfus	5.39	kJ/mol	Joback Method
hvap	31.98	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.342		Crippen Method
mcvol	56.200	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	392.00		NIST Webbook
rinpol	392.00		NIST Webbook
tb	379.98	K	Joback Method
tc	574.02	K	Joback Method
tf	210.81	K	Joback Method
vc	0.247	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	92.00	J/mol×K	379.98	Joback Method
cpg	95.56	J/mol×K	412.32	Joback Method
cpg	98.80	J/mol×K	444.66	Joback Method
cpg	101.72	J/mol×K	477.00	Joback Method
cpg	104.35	J/mol×K	509.34	Joback Method
cpg	106.72	J/mol×K	541.68	Joback Method

cpg	108.83	J/mol×K	574.02	Joback Method

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=C421056&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume