Acetonitrile, dichlorofluoro-

Other names: Dichlorofluoro acetonitrile
Inchi: InChI=1S/C2Cl2FN/c3-2(4,5)1-6
InchiKey: IUHXUTRMGQCBPC-UHFFFAOYSA-N
Formula: C2Cl2FN
SMILES: N#CC(F)(Cl)Cl
Mol. weight [g/mol]: 127.93
CAS: 353-82-2

Physical Properties

Property code	Value	Unit	Source
gf	-116.69	kJ/mol	Joback Method
hf	-156.07	kJ/mol	Joback Method
hfus	6.50	kJ/mol	Joback Method
hvap	37.18	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.611		Crippen Method
mcvol	66.670	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	418.14	K	Joback Method
tc	632.12	K	Joback Method
tf	240.14	K	Joback Method
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.43	J/mol×K	418.14	Joback Method
cpg	103.68	J/mol×K	453.80	Joback Method
cpg	106.56	J/mol×K	489.47	Joback Method
cpg	109.10	J/mol×K	525.13	Joback Method
cpg	111.33	J/mol×K	560.79	Joback Method
cpg	113.28	J/mol×K	596.45	Joback Method
cpg	114.97	J/mol×K	632.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C353822&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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