2-CHLORO-6-FLUOROPHENYLACETONITRILE

Other names: 2-Chloro-6-fluorophenylacetonitrile
Benzeneacetonitrile, 2-chloro-6-fluoro-
Inchi: InChI=1S/C8H5ClFN/c9-7-2-1-3-8(10)6(7)4-5-11/h1-3H,4H2
InchiKey: ZGSAFMIRVLOISC-UHFFFAOYSA-N
Formula: C8H5ClFN
SMILES: N#CCc1c(F)cccc1Cl
Mol. weight [g/mol]: 169.59

Physical Properties

Property code	Value	Unit	Source
hfus	18.52	kJ/mol	Joback Method
ie	9.58	eV	Cheméo Relay (1.0)
log10ws	-2.89		Cheméo Relay (1.0)
logp	2.545		Crippen Method
mcvol	115.210	ml/mol	McGowan Method
tb	508.82	K	Cheméo Relay (1.0)
tf	363.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.97	J/mol×K	557.86	Joback Method
cpg	238.45	J/mol×K	595.61	Joback Method
cpg	246.38	J/mol×K	633.35	Joback Method
cpg	253.78	J/mol×K	671.10	Joback Method
cpg	260.68	J/mol×K	708.85	Joback Method
cpg	267.09	J/mol×K	746.59	Joback Method
cpg	273.04	J/mol×K	784.34	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75279559&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point