

C7H7ClFN

Inchi:	InChI=1S/C7H7ClFN/c8-7-3-6(9)2-1-5(7)4-10/h1-3H,4,10H2
InchiKey:	CBKWAXKMZUULLO-UHFFFAOYSA-N
Formula:	C7H7ClFN
SMILES:	NCc1ccc(F)cc1Cl
Mol. weight [g/mol]:	159.59
CAS:	15205-11-5

Physical Properties

Property code	Value	Unit	Source
gf	-39.08	kJ/mol	Joback Method
hf	-152.28	kJ/mol	Joback Method
hfus	19.62	kJ/mol	Joback Method
hvap	48.98	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.938		Crippen Method
mcvol	109.720	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
tb	505.43	K	Joback Method
tc	728.11	K	Joback Method
tf	333.88	K	Joback Method
vc	0.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.46	J/mol×K	505.43	Joback Method
cpg	229.16	J/mol×K	542.54	Joback Method
cpg	238.28	J/mol×K	579.66	Joback Method
cpg	246.82	J/mol×K	616.77	Joback Method
cpg	254.82	J/mol×K	653.88	Joback Method
cpg	262.29	J/mol×K	691.00	Joback Method
cpg	269.27	J/mol×K	728.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15205115&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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