

1-Chloro-3,5-difluorobenzene

Other names:	1-Chloro-3,5-difluorobenzene
Inchi:	InChI=1S/C6H3ClF2/c7-4-1-5(8)3-6(9)2-4/h1-3H
InchiKey:	RFKBODCWHNDUTJ-UHFFFAOYSA-N
Formula:	C6H3ClF2
SMILES:	Fc1cc(F)cc(Cl)c1
Mol. weight [g/mol]:	148.54

Physical Properties

Property code	Value	Unit	Source
hf	-302.34	kJ/mol	Cheméo Relay (1.0)
hfus	14.92	kJ/mol	Joback Method
hvap	42.23	kJ/mol	Cheméo Relay (1.0)
ie	9.40 ± 0.02	eV	NIST Webbook
log10ws	-2.92		Cheméo Relay (1.0)
logp	2.618		Crippen Method
mcvol	87.420	ml/mol	McGowan Method
tb	394.58	K	Cheméo Relay (1.0)
tf	252.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.97	J/mol×K	409.29	Joback Method
cpg	152.39	J/mol×K	442.79	Joback Method
cpg	159.40	J/mol×K	476.29	Joback Method
cpg	166.03	J/mol×K	509.79	Joback Method
cpg	172.28	J/mol×K	543.29	Joback Method
cpg	178.17	J/mol×K	576.79	Joback Method
cpg	183.71	J/mol×K	610.29	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1435434&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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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

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