

Cyclohexane, fluoro-

Other names:	Cyclohexyl fluoride Fluorocyclohexane
Inchi:	InChI=1S/C6H11F/c7-6-4-2-1-3-5-6/h6H,1-5H2
InchiKey:	GOBGVVAHHOUMDK-UHFFFAOYSA-N
Formula:	C6H11F
SMILES:	FC1CCCCC1
Mol. weight [g/mol]:	102.15
CAS:	372-46-3

Physical Properties

Property code	Value	Unit	Source
chl	-3738.59 ± 0.84	kJ/mol	NIST Webbook
gf	-170.72	kJ/mol	Joback Method
hf	-336.60 ± 1.10	kJ/mol	NIST Webbook
hfl	-374.06 ± 0.84	kJ/mol	NIST Webbook
hfus	6.21	kJ/mol	Joback Method
hvap	37.50 ± 0.30	kJ/mol	NIST Webbook
hvap	37.45 ± 0.73	kJ/mol	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.289		Crippen Method
mcvol	86.310	ml/mol	McGowan Method
pc	5172.59 ± 100.00	kPa	NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	738.00		NIST Webbook
ripol	958.00		NIST Webbook
ripol	990.00		NIST Webbook
ripol	990.00		NIST Webbook
ripol	958.00		NIST Webbook
tb	355.50	K	Joback Method
tc	667.93 ± 3.00	K	NIST Webbook
tf	165.35	K	Joback Method
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.10	J/mol×K	483.47	Joback Method
cpg	206.76	J/mol×K	515.47	Joback Method
cpg	142.34	J/mol×K	355.50	Joback Method
cpg	156.48	J/mol×K	387.49	Joback Method
cpg	169.97	J/mol×K	419.49	Joback Method
cpg	182.84	J/mol×K	451.48	Joback Method
cpg	217.84	J/mol×K	547.46	Joback Method
hfust	2.58	kJ/mol	285.30	NIST Webbook
hvapt	35.00	kJ/mol	344.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C372463&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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