

Naphthalene, 1-fluoro-

Other names:	1-Fluornaftalen 1-Fluoronaphthalene ALPHA-FLUORONAPHTHALENE «alpha»-Fluoronaphthalene Â«alphaÂ»-Fluoronaphthalene
Inchi:	InChI=1S/C10H7F/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H
InchiKey:	CWLKTJOTWITYSI-UHFFFAOYSA-N
Formula:	C10H7F
SMILES:	Fc1cccc2ccccc12
Mol. weight [g/mol]:	146.16
CAS:	321-38-0

Physical Properties

Property code	Value	Unit	Source
chl	-5096.00 ± 92.00	kJ/mol	NIST Webbook
gf	47.94	kJ/mol	Joback Method
hf	-29.71	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	41.61	kJ/mol	Joback Method
ie	8.15	eV	NIST Webbook
log10ws	-3.61		Crippen Method
logp	2.979		Crippen Method
mvol	110.310	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
rinpol	200.11		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1162.50		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	200.19		NIST Webbook
rinpol	1207.00		NIST Webbook
ripol	198.43		NIST Webbook
ripol	1715.00		NIST Webbook
tb	488.20	K	NIST Webbook
tb	489.00 ± 1.00	K	NIST Webbook
tc	704.04	K	Joback Method

tf	274.69	K	Joback Method
vc	0.427	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.17	J/mol×K	478.11	Joback Method
cpg	230.76	J/mol×K	515.77	Joback Method
cpg	242.41	J/mol×K	553.42	Joback Method
cpg	253.16	J/mol×K	591.08	Joback Method
cpg	263.09	J/mol×K	628.73	Joback Method
cpg	272.26	J/mol×K	666.39	Joback Method
cpg	280.72	J/mol×K	704.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	1.50	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.therc.org/files/research/kdb/mol/mol1711.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C321380&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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