

1H-Inden-1-one, 5-fluoro-2,3-dihydro-

Other names:	5-FLUOROINDANONE
Inchi:	InChI=1S/C9H7FO/c10-7-2-3-8-6(5-7)1-4-9(8)11/h2-3,5H,1,4H2
InchiKey:	WVPPBVAMKNQXJA-UHFFFAOYSA-N
Formula:	C9H7FO
SMILES:	O=C1CCc2cc(F)ccc21
Mol. weight [g/mol]:	150.15
CAS:	700-84-5

Physical Properties

Property code	Value	Unit	Source
gf	-130.89	kJ/mol	Joback Method
hf	-256.17	kJ/mol	Joback Method
hfus	11.98	kJ/mol	Joback Method
hvap	42.88	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	1.955		Crippen Method
mcvol	106.390	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	520.46	K	Joback Method
tc	753.82	K	Joback Method
tf	333.64	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.21	J/mol×K	520.46	Joback Method
cpg	244.59	J/mol×K	559.35	Joback Method
cpg	256.19	J/mol×K	598.25	Joback Method
cpg	267.05	J/mol×K	637.14	Joback Method
cpg	277.19	J/mol×K	676.04	Joback Method
cpg	286.66	J/mol×K	714.93	Joback Method
cpg	295.47	J/mol×K	753.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C700845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mcvol:	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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