

Hexane, 2-fluoro-

Inchi:	InChI=1S/C6H13F/c1-3-4-5-6(2)7/h6H,3-5H2,1-2H3
InchiKey:	KDSVEERUTJJIEW-UHFFFAOYSA-N
Formula:	C6H13F
SMILES:	CCCCC(C)F
Mol. weight [g/mol]:	104.17
CAS:	372-54-3

Physical Properties

Property code	Value	Unit	Source
gf	-197.61	kJ/mol	Joback Method
hf	-368.56	kJ/mol	Joback Method
hfus	10.85	kJ/mol	Joback Method
hvap	27.75	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.535		Crippen Method
mcvol	97.170	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpola	668.00		NIST Webbook
tb	335.51	K	Joback Method
tc	493.52	K	Joback Method
tf	142.97	K	Joback Method
vc	0.384	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.51	J/molxK	335.51	Joback Method
cpg	176.80	J/molxK	361.84	Joback Method
cpg	186.74	J/molxK	388.18	Joback Method
cpg	196.33	J/molxK	414.51	Joback Method
cpg	205.60	J/molxK	440.85	Joback Method
cpg	214.54	J/molxK	467.18	Joback Method
cpg	223.15	J/molxK	493.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C372543&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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