

Isobutyl fluoride

Inchi:

InChI=1S/C4H9F/c1-4(2)3-5/h4H,3H2,1-2H3

InchiKey:

WGCJTTUVWKJDAX-UHFFFAOYSA-N

Formula:

C4H9F

SMILES:

CC(C)CF

Mol. weight [g/mol]:

76.11

Physical Properties

Property code	Value	Unit	Source
gf	-214.45	kJ/mol	Joback Method
hf	-327.28	kJ/mol	Joback Method
hfus	5.67	kJ/mol	Joback Method
hvap	23.29	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	1.612		Crippen Method
mcvol	68.990	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	442.00		NIST Webbook
tb	289.75	K	Joback Method
tc	445.48	K	Joback Method
tf	120.43	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.10	J/mol×K	289.75	Joback Method
cpg	110.47	J/mol×K	315.70	Joback Method
cpg	117.60	J/mol×K	341.66	Joback Method
cpg	124.50	J/mol×K	367.61	Joback Method
cpg	131.17	J/mol×K	393.57	Joback Method
cpg	137.62	J/mol×K	419.52	Joback Method
cpg	143.86	J/mol×K	445.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511863&Units=SI

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
hvac:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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