

Butane, 1-fluoro-3,3-dimethyl

Inchi:	InChI=1S/C5H11F/c1-5(2)3-4-6/h5H,3-4H2,1-2H3
InchiKey:	TVHQEXCGMKZBME-UHFFFAOYSA-N
Formula:	C5H11F
SMILES:	CC(C)CCF
Mol. weight [g/mol]:	90.14

Physical Properties

Property code	Value	Unit	Source
gf	-206.03	kJ/mol	Joback Method
hf	-347.92	kJ/mol	Joback Method
hfus	8.26	kJ/mol	Joback Method
hvap	25.52	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	2.002		Crippen Method
mcvol	83.080	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinpol	637.00		NIST Webbook
tb	312.63	K	Joback Method
tc	469.78	K	Joback Method
tf	131.70	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.44	J/molxK	312.63	Joback Method
cpg	142.32	J/molxK	338.82	Joback Method
cpg	150.91	J/molxK	365.01	Joback Method
cpg	159.21	J/molxK	391.20	Joback Method
cpg	167.23	J/molxK	417.40	Joback Method
cpg	174.98	J/molxK	443.59	Joback Method
cpg	182.45	J/molxK	469.78	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=R511398&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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