

Benzene, 1-fluoro-3-ethyl

Inchi:	InChI=1S/C8H9F/c1-2-7-4-3-5-8(9)6-7/h3-6H,2H2,1H3
InchiKey:	ZEWGMOQWTWMZMZ-UHFFFAOYSA-N
Formula:	C8H9F
SMILES:	CCc1cccc(F)c1
Mol. weight [g/mol]:	124.16

Physical Properties

Property code	Value	Unit	Source
gf	-75.55	kJ/mol	Joback Method
hf	-179.50	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	35.52	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.388		Crippen Method
mvol	101.590	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	879.00		NIST Webbook
rinpol	879.00		NIST Webbook
tb	413.37	K	Joback Method
tc	612.69	K	Joback Method
tf	219.45	K	Joback Method
vc	0.394	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.90	J/mol×K	413.37	Joback Method
cpg	196.54	J/mol×K	446.59	Joback Method
cpg	207.57	J/mol×K	479.81	Joback Method
cpg	218.03	J/mol×K	513.03	Joback Method
cpg	227.93	J/mol×K	546.25	Joback Method
cpg	237.29	J/mol×K	579.47	Joback Method
cpg	246.13	J/mol×K	612.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R636318&Units=SI
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

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

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