Benzene, 2-fluoro-1,3,5-trimethyl-

Other names: 1-Fluoro-2,4,6-trimethylbenzene
Inchi: InChI=1S/C9H11F/c1-6-4-7(2)9(10)8(3)5-6/h4-5H,1-3H3
InchiKey: ZLGPNBBJPOBSLY-UHFFFAOYSA-N
Formula: C9H11F
SMILES: Cc1cc(C)c(F)c(C)c1
Mol. weight [g/mol]: 138.18
CAS: 392-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-86.39	kJ/mol	Joback Method
hf	-223.08	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	39.07	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.751		Crippen Method
mcvol	115.680	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
ripol	2134.00		NIST Webbook
tb	444.70	K	NIST Webbook
tc	646.28	K	Joback Method
tf	255.76	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.90	J/mol×K	446.21	Joback Method
cpg	237.83	J/mol×K	479.56	Joback Method
cpg	249.24	J/mol×K	512.90	Joback Method
cpg	260.13	J/mol×K	546.25	Joback Method
cpg	270.51	J/mol×K	579.59	Joback Method
cpg	280.40	J/mol×K	612.94	Joback Method
cpg	289.81	J/mol×K	646.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C392698&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume