

Benzenamine, 4-fluoro-2-methyl-

Other names:	4-Fluoro-2-methylaniline 3-Fluoro-6-aminotoluene 2-Amino-5-fluorotoluene o-Toluidine, 4-fluoro- 6-Amino-3-fluorotoluene 4-Fluoro-2-methylbenzenamine 2-Methyl-4-fluoroaniline 4-fluorotoluidine
Inchi:	InChI=1S/C7H8FN/c1-5-4-6(8)2-3-7(5)9/h2-4H,9H2,1H3
InchiKey:	KMHLGVTVACLEJE-UHFFFAOYSA-N
Formula:	C7H8FN
SMILES:	Cc1cc(F)ccc1N
Mol. weight [g/mol]:	125.14
CAS:	452-71-1

Physical Properties

Property code	Value	Unit	Source
gf	-27.15	kJ/mol	Joback Method
hf	-136.54	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	59.80 ± 0.80	kJ/mol	NIST Webbook
log10ws	-1.91		Crippen Method
logp	1.716		Crippen Method
mcvol	97.480	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	468.00	K	Joback Method
tc	685.00	K	Joback Method
tf	303.96	K	Joback Method
vc	0.366	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.53	J/mol×K	468.00	Joback Method

cpg	206.84	J/mol×K	504.17	Joback Method
cpg	216.58	J/mol×K	540.33	Joback Method
cpg	225.78	J/mol×K	576.50	Joback Method
cpg	234.45	J/mol×K	612.66	Joback Method
cpg	242.60	J/mol×K	648.83	Joback Method
cpg	250.26	J/mol×K	685.00	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.20	K	2.10	NIST Webbook
tbrp	364.00 ± 1.00	K	2.10	NIST Webbook
tbrp	367.20	K	2.10	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C452711&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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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