3-FLUORO-2-METHYLANILINE

Other names: 6-Amino-2-fluorotoluene
Benzenamine, 3-fluoro-2-methyl-
3-fluoro-o-toluidine
Inchi: InChI=1S/C7H8FN/c1-5-6(8)3-2-4-7(5)9/h2-4H,9H2,1H3
InchiKey: SLDLVGFPFFLYBM-UHFFFAOYSA-N
Formula: C7H8FN
SMILES: Cc1c(N)cccc1F
Mol. weight [g/mol]: 125.15

Physical Properties

Property code	Value	Unit	Source
hf	-168.94	kJ/mol	Cheméo Relay (1.0)
hfus	15.43	kJ/mol	Joback Method
hvap	57.80 ± 0.60	kJ/mol	NIST Webbook
ie	8.05	eV	Cheméo Relay (1.0)
log10ws	-1.33		Cheméo Relay (1.0)
logp	1.716		Crippen Method
mcvol	97.480	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	474.51	K	Cheméo Relay (1.0)
tc	693.93	K	Cheméo Relay (1.0)
tf	300.09	K	Cheméo Relay (1.0)

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

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C443867&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point