

2-FLUORO-4-METHYLANILINE

Other names:	p-Toluidine, 2-fluoro- Benzenamine, 2-fluoro-4-methyl- 2-Fluoro-p-toluidine 4-Amino-3-fluorotoluene
Inchi:	InChI=1S/C7H8FN/c1-5-2-3-7(9)6(8)4-5/h2-4H,9H2,1H3
InchiKey:	ZQEXBVHABAJPHJ-UHFFFAOYSA-N
Formula:	C7H8FN
SMILES:	Cc1ccc(N)c(F)c1
Mol. weight [g/mol]:	125.15

Physical Properties

Property code	Value	Unit	Source
af	0.4384		Cheméo Relay (1.0)
hfus	15.43	kJ/mol	Joback Method
hvap	56.60 ± 0.60	kJ/mol	NIST Webbook
ie	7.95	eV	Cheméo Relay (1.0)
logp	1.716		Crippen Method
mcvol	97.480	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	459.75	K	Cheméo Relay (1.0)
tc	691.74	K	Cheméo Relay (1.0)
tf	310.71	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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C452802&Units=SI>

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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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