P-FLUORO-N,N-DIMETHYLANILINE

Other names: N,N-Dimethyl-4-fluoroaniline
Inchi: InChI=1S/C8H10FN/c1-10(2)8-5-3-7(9)4-6-8/h3-6H,1-2H3
InchiKey: YJEHCGOJNJUOII-UHFFFAOYSA-N
Formula: C8H10FN
SMILES: CN(C)c1ccc(F)cc1
Mol. weight [g/mol]: 139.17

Physical Properties

Property code	Value	Unit	Source
af	0.3970		Cheméo Relay (1.0)
affp	924.80	kJ/mol	NIST Webbook
basg	898.30	kJ/mol	NIST Webbook
gf	35.23	kJ/mol	Joback Method
hf	-128.35	kJ/mol	Cheméo Relay (1.0)
hfus	16.23	kJ/mol	Joback Method
hvap	53.25	kJ/mol	Cheméo Relay (1.0)
ie	7.50	eV	NIST Webbook
log10ws	-2.02		Cheméo Relay (1.0)
logp	1.892		Crippen Method
mcvol	111.570	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	463.38	K	Cheméo Relay (1.0)
tc	665.60	K	Cheméo Relay (1.0)
tf	295.34	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.88	J/mol×K	425.81	Joback Method
cpg	226.68	J/mol×K	458.65	Joback Method
cpg	238.77	J/mol×K	491.49	Joback Method
cpg	250.18	J/mol×K	524.33	Joback Method
cpg	260.93	J/mol×K	557.17	Joback Method
cpg	271.05	J/mol×K	590.01	Joback Method

cpg	280.58	J/mol×K	622.84	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C403463&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

Cheméo Relay (1.0):

Legend

af: Acentric Factor
affp: Proton affinity
basg: Gas basicity
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
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