2,4-DIFLUOROANISOLE

Other names: Benzene, 2,4-difluoro-1-methoxy-
Inchi: InChI=1S/C7H6F2O/c1-10-7-3-2-5(8)4-6(7)9/h2-4H,1H3
InchiKey: CRMJLJFDPNJIQA-UHFFFAOYSA-N
Formula: C7H6F2O
SMILES: COc1ccc(F)cc1F
Mol. weight [g/mol]: 144.12

Physical Properties

Property code	Value	Unit	Source
hfus	14.50	kJ/mol	Joback Method
hvap	48.42	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	1.973		Crippen Method
mcvol	95.140	ml/mol	McGowan Method
tb	424.00	K	NIST Webbook
tf	269.34	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.52	J/mol×K	417.16	Joback Method
cpg	187.48	J/mol×K	449.01	Joback Method
cpg	196.09	J/mol×K	480.86	Joback Method
cpg	204.36	J/mol×K	512.71	Joback Method
cpg	212.29	J/mol×K	544.55	Joback Method
cpg	219.87	J/mol×K	576.40	Joback Method
cpg	227.11	J/mol×K	608.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	326.20	K	2.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C452108&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):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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