2,6-DIFLUOROPHENOL

Other names: phenol, 2,6-difluoro-
Inchi: InChI=1S/C6H4F2O/c7-4-2-1-3-5(8)6(4)9/h1-3,9H
InchiKey: CKKOVFGIBXCEIJ-UHFFFAOYSA-N
Formula: C6H4F2O
SMILES: Oc1c(F)cccc1F
Mol. weight [g/mol]: 130.09

Physical Properties

Property code	Value	Unit	Source
hf	-465.61	kJ/mol	Cheméo Relay (1.0)
hfus	77.80	kJ/mol	Calorimetric and computational thermochemical study of difluorophenol isomers
hsub	77.80 ± 2.00	kJ/mol	NIST Webbook
hvap	56.15	kJ/mol	Cheméo Relay (1.0)
ie	8.83	eV	Cheméo Relay (1.0)
log10ws	-0.97		Cheméo Relay (1.0)
logp	1.670		Crippen Method
mcvol	81.050	ml/mol	McGowan Method
tb	411.06	K	Cheméo Relay (1.0)
tc	650.99	K	Cheméo Relay (1.0)
tf	302.08	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.73	J/mol×K	447.50	Joback Method
cpg	170.76	J/mol×K	482.47	Joback Method
cpg	178.16	J/mol×K	517.44	Joback Method
cpg	184.98	J/mol×K	552.41	Joback Method
cpg	191.27	J/mol×K	587.38	Joback Method
cpg	197.08	J/mol×K	622.35	Joback Method
cpg	202.48	J/mol×K	657.32	Joback Method

Sources

Calorimetric and computational thermochemical study of difluorophenol isomers:	https://www.doi.org/10.1016/j.jct.2009.07.011
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28177482&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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
tc:	Critical Temperature
tf:	Normal melting (fusion) point