2,5-Difluorophenol

Other names: Phenol,2,5-difluoro-
Inchi: InChI=1S/C6H4F2O/c7-4-1-2-5(8)6(9)3-4/h1-3,9H
InchiKey: INXKVYFOWNAVMU-UHFFFAOYSA-N
Formula: C6H4F2O
SMILES: Oc1cc(F)ccc1F
Mol. weight [g/mol]: 130.09
CAS: 2713-31-7

Physical Properties

Property code	Value	Unit	Source
gf	-441.82	kJ/mol	Joback Method
hf	-511.64	kJ/mol	Joback Method
hfus	16.89	kJ/mol	Joback Method
hsub	68.00 ± 1.40	kJ/mol	NIST Webbook
hvap	43.27	kJ/mol	Joback Method
ie	9.10 ± 0.02	eV	NIST Webbook
log10ws	-1.68		Crippen Method
logp	1.670		Crippen Method
mcvol	81.050	ml/mol	McGowan Method
pc	4966.33	kPa	Joback Method
tb	447.50	K	Joback Method
tc	657.32	K	Joback Method
tf	309.22	K	Joback Method
vc	0.266	m3/kmol	Joback Method

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2713317&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume