Phenol-d6-

Other names: (2H6)phenol
Inchi: InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H/i1D,2D,3D,4D,5D/hD
InchiKey: ISWSIDIOOBJBQZ-QNKSCLMFSA-N
Formula: C6D6O
SMILES: Oc1ccccc1
Mol. weight [g/mol]: 100.15
CAS: 13127-88-3

Physical Properties

Property code	Value	Unit	Source
gf	-32.94	kJ/mol	Joback Method
hf	-96.48	kJ/mol	Joback Method
hfus	11.51	kJ/mol	Joback Method
hvap	43.58	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	1.392		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
pc	5926.27	kPa	Joback Method
tb	439.00	K	Joback Method
tc	671.01	K	Joback Method
tf	283.00	K	Joback Method
vc	0.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.52	J/mol×K	439.00	Joback Method
cpg	187.47	J/mol×K	632.34	Joback Method
cpg	180.59	J/mol×K	593.67	Joback Method
cpg	173.03	J/mol×K	555.01	Joback Method
cpg	164.73	J/mol×K	516.34	Joback Method
cpg	155.59	J/mol×K	477.67	Joback Method
cpg	193.78	J/mol×K	671.01	Joback Method
dvisc	0.0001736	Pa×s	439.00	Joback Method

dvisc	0.0002857	Pa×s	413.00	Joback Method
dvisc	0.0005026	Pa×s	387.00	Joback Method
dvisc	0.0009592	Pa×s	361.00	Joback Method
dvisc	0.0020238	Pa×s	335.00	Joback Method
dvisc	0.0048418	Pa×s	309.00	Joback Method
dvisc	0.0135969	Pa×s	283.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13127883&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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