3-Hydroxyphenylacetylene

Inchi: InChI=1S/C8H6O/c1-2-7-4-3-5-8(9)6-7/h1,3-6,9H
InchiKey: AODMJIOEGCBUQL-UHFFFAOYSA-N
Formula: C8H6O
SMILES: C#Cc1cccc(O)c1
Mol. weight [g/mol]: 118.13
CAS: 10401-11-3

Physical Properties

Property code	Value	Unit	Source
gf	197.34	kJ/mol	Joback Method
hf	142.67	kJ/mol	Joback Method
hfus	19.27	kJ/mol	Joback Method
hvap	48.55	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.373		Crippen Method
mcvol	97.090	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
tb	479.86	K	Joback Method
tc	723.96	K	Joback Method
tf	365.03	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.18	J/mol×K	479.86	Joback Method
cpg	203.21	J/mol×K	520.54	Joback Method
cpg	212.28	J/mol×K	561.23	Joback Method
cpg	220.51	J/mol×K	601.91	Joback Method
cpg	228.00	J/mol×K	642.59	Joback Method
cpg	234.86	J/mol×K	683.28	Joback Method
cpg	241.18	J/mol×K	723.96	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=C10401113&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
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