4-Ethylcatechol

Other names: 1,2-Benzenediol, 4-ethyl-
4-ethylpyrocatechol
Inchi: InChI=1S/C8H10O2/c1-2-6-3-4-7(9)8(10)5-6/h3-5,9-10H,2H2,1H3
InchiKey: HFLGBNBLMBSXEM-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: CCc1ccc(O)c(O)c1
Mol. weight [g/mol]: 138.16
CAS: 1124-39-6

Physical Properties

Property code	Value	Unit	Source
gf	-180.35	kJ/mol	Joback Method
hf	-326.54	kJ/mol	Joback Method
hfus	22.08	kJ/mol	Joback Method
hvap	61.71	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.660		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	5430.51	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	570.36	K	Joback Method
tc	808.73	K	Joback Method
tf	429.78	K	Joback Method
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.81	J/mol×K	570.36	Joback Method
cpg	280.11	J/mol×K	610.09	Joback Method
cpg	289.56	J/mol×K	649.82	Joback Method
cpg	298.31	J/mol×K	689.55	Joback Method
cpg	306.50	J/mol×K	729.28	Joback Method

cpg	314.26	J/mol×K	769.01	Joback Method
cpg	321.75	J/mol×K	808.73	Joback Method
dvisc	0.0003550	Pa×s	429.78	Joback Method
dvisc	0.0001700	Pa×s	453.21	Joback Method
dvisc	0.0000875	Pa×s	476.64	Joback Method
dvisc	0.0000479	Pa×s	500.07	Joback Method
dvisc	0.0000277	Pa×s	523.50	Joback Method
dvisc	0.0000168	Pa×s	546.93	Joback Method
dvisc	0.0000106	Pa×s	570.36	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1124396&Units=SI

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume