

1,3-Benzenediol, 4-ethyl-

Other names:	1,3-Dihydroxy-4-ethylbenzene 2,4-Dihydroxy-1-ethylbenzene 4 Ethyl 1,3-benzenediol 4-Ethylresorcinol 6-Ethylresorcinol Resorcinol, 4-ethyl-
Inchi:	InChI=1S/C8H10O2/c1-2-6-3-4-7(9)5-8(6)10/h3-5,9-10H,2H2,1H3
InchiKey:	VGMJYYDKPUPTID-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	CCc1ccc(O)cc1O
Mol. weight [g/mol]:	138.16
CAS:	2896-60-8

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	1314.00		NIST Webbook
rinpol	1314.00		NIST Webbook
tb	570.36	K	Joback Method
tc	808.73	K	Joback Method
tf	370.40	K	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.81	J/molxK	570.36	Joback Method
cpg	280.11	J/molxK	610.09	Joback Method
cpg	289.56	J/molxK	649.82	Joback Method
cpg	298.31	J/molxK	689.55	Joback Method
cpg	306.50	J/molxK	729.28	Joback Method
cpg	314.26	J/molxK	769.01	Joback Method
cpg	321.75	J/molxK	808.73	Joback Method
dvisc	0.0003550	Paxs	429.78	Joback Method
dvisc	0.0001700	Paxs	453.21	Joback Method
dvisc	0.0000875	Paxs	476.64	Joback Method
dvisc	0.0000479	Paxs	500.07	Joback Method
dvisc	0.0000277	Paxs	523.50	Joback Method
dvisc	0.0000168	Paxs	546.93	Joback Method
dvisc	0.0000106	Paxs	570.36	Joback Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Vapour pressure data for
2-n-propylresorcinol, 4-ethylresorcinol
and 4-hexylresorcinol near their normal
boiling points measured by differential
scanning calorimetry:

<https://www.doi.org/10.1016/j.jct.2019.03.008>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2896608&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

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