Hexylresorcinol

Other names:	1,3-Benzenediol, 4-hexyl-
	1,3-Dihydroxy-4-Hexylbenzene
	1,3-Dihydroxy-4-n-hexylbenzene
	1-(2',4'-Dihydroxyphenyl)hexane
	4-(1-Hexyl)resorcinol
	4-Hexyl-1,3-benzenediol
	4-Hexyl-1,3-dihydroxybenzene
	4-Hexylresorcine
	4-Hexylresorcinol
	4-hexylbenzene, 1,3-dihydroxy-
	4-n-Hexylresorcinol
	Adrover
	Antascarin
	Ascaricid
	Ascarinol
	Ascaryl
	Caprokol
	Crystoids
	Cystoids Anthelmintic
	Gelovermin
	Hexylresorcin
	Hidesol
	Mycoderm
	NCI-C55787
	NSC 1570
	Oxana
	Prensol
	Resorcinol, 4-hexyl-
	S.T. 37
	ST-37
	Sucrets
	Worm-agen
	benzene, 4-hexyl-1,3-dihydroxy-
	p-Hexylresorcinol
Inchi:	InChI=1S/C12H18O2/c1-2-3-4-5-6-10-7-8-11(13)9-12(10)14/h7-9,13-14H,2-6H2,1H3
InchiKey:	WFJIVOKAWHGMBH-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CCCCCCc1ccc(O)cc1O
Mol. weight [g/mol]:	194.27
CAS:	136-77-6

Physical Properties

Property code	Value	Unit	Source
gf	-146.67	kJ/mol	Joback Method
hf	-409.10	kJ/mol	Joback Method
hfus	32.44	kJ/mol	Joback Method
hvap	70.61	kJ/mol	Joback Method
log10ws	-2.59		Aqueous Solubility Prediction Method
log10ws	-2.59		Estimated Solubility Method
logp	3.221		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	1777.00		NIST Webbook
tb	607.20	K	NIST Webbook
tc	882.46	K	Joback Method
tf	339.48	K	Aqueous Solubility Prediction Method
tf	340.10	K	Vapour pressure data for 2-n-propylresorcinol, 4-ethylresorcinol and 4-hexylresorcinol near their normal boiling points measured by differential scanning calorimetry
tf	341.00 ± 0.10	K	NIST Webbook
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.35	J/mol×K	808.94	Joback Method
cpg	530.34	J/mol×K	882.46	Joback Method
cpg	519.48	J/mol×K	845.70	Joback Method
cpg	458.64	J/mol×K	661.88	Joback Method
cpg	472.10	J/mol×K	698.64	Joback Method
cpg	484.79	J/mol×K	735.41	Joback Method
cpg	496.83	J/mol×K	772.17	Joback Method
dvisc	0.0000027	Pa×s	661.88	Joback Method

dvisc	0.0000075	Pa×s	599.54	Joback Method
dvisc	0.0000044	Pa×s	630.71	Joback Method
dvisc	0.0001287	Pa×s	474.86	Joback Method
dvisc	0.0000554	Pa×s	506.03	Joback Method
dvisc	0.0000263	Pa×s	537.20	Joback Method
dvisc	0.0000135	Pa×s	568.37	Joback Method
hfust	19.04	kJ/mol	341.50	NIST Webbook
hfust	19.04	kJ/mol	341.50	NIST Webbook
hvapt	88.10	kJ/mol	464.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	452.20	K	0.80	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C136776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/85-693-9/Hexylresorcinol.pdf

Generated by Cheméo on 2025-12-05 22:43:35.984271077 +0000 UTC m=+4722813.514311732.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.