

1,3-Benzenediol, 5-pentyl-

Other names:	Olivetol Resorcinol, 5-pentyl- 5-n-Amylresorcinol 3,5-Dihydroxyamylbenzene 5-Pentylresorcinol 5-n-Pentylresorcinol
Inchi:	InChI=1S/C11H16O2/c1-2-3-4-5-9-6-10(12)8-11(13)7-9/h6-8,12-13H,2-5H2,1H3
InchiKey:	IRMPFYJSHJGOPE-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	CCCCCc1cc(O)cc(O)c1
Mol. weight [g/mol]:	180.24
CAS:	500-66-3

Physical Properties

Property code	Value	Unit	Source
gf	-155.09	kJ/mol	Joback Method
hf	-388.46	kJ/mol	Joback Method
hfus	29.85	kJ/mol	Joback Method
hvap	68.38	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.830		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1770.80		NIST Webbook
rinpol	1770.80		NIST Webbook
tb	639.00	K	Joback Method
tc	863.62	K	Joback Method
tf	463.59	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.13	J/molxK	639.00	Joback Method
cpg	421.92	J/molxK	676.44	Joback Method
cpg	433.93	J/molxK	713.87	Joback Method
cpg	445.26	J/molxK	751.31	Joback Method
cpg	456.06	J/molxK	788.74	Joback Method
cpg	466.46	J/molxK	826.18	Joback Method
cpg	476.57	J/molxK	863.62	Joback Method
dvisc	0.0001659	Paxs	463.59	Joback Method
dvisc	0.0000731	Paxs	492.82	Joback Method
dvisc	0.0000353	Paxs	522.06	Joback Method
dvisc	0.0000184	Paxs	551.29	Joback Method
dvisc	0.0000103	Paxs	580.53	Joback Method
dvisc	0.0000060	Paxs	609.76	Joback Method
dvisc	0.0000037	Paxs	639.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C500663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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