1,3-Dihydroxy-4-pentylbenzene

Inchi: InChI=1S/C11H16O2/c1-2-3-4-5-9-6-7-10(12)8-11(9)13/h6-8,12-13H,2-5H2,1H3
InchiKey: PJHYOCWMKYASAB-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CCCCCc1ccc(O)cc1O
Mol. weight [g/mol]: 180.24
CAS: 533-24-4

Physical Properties

Property code	Value	Unit	Source
hfus	29.85	kJ/mol	Joback Method
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-3.12		Cheméo Relay (1.0)
logp	2.830		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
rinpol	1710.60		NIST Webbook
rinpol	1710.60		NIST Webbook
tb	579.27	K	Cheméo Relay (1.0)
tf	345.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	84.90	kJ/mol	455.50	NIST Webbook

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$

Y unit	J/mol×K
Coeff. A	-5.88560e+01
Coeff. B	1.27912e+00
Coeff. C	-1.11852e-03
Coeff. D	4.11400e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-2.25207e+01
Coeff. B	6.40518e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	345.65
Temperature range (K), max.	604.72

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C533244&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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