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
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	1710.60		NIST Webbook
rinpol	1710.60		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/mol×K	639.00	Joback Method
cpg	421.92	J/mol×K	676.44	Joback Method
cpg	433.93	J/mol×K	713.87	Joback Method
cpg	445.26	J/mol×K	751.31	Joback Method
cpg	456.06	J/mol×K	788.74	Joback Method
cpg	466.46	J/mol×K	826.18	Joback Method
cpg	476.57	J/mol×K	863.62	Joback Method

dvisc	0.0001659	Pa×s	463.59	Joback Method
dvisc	0.0000731	Pa×s	492.82	Joback Method
dvisc	0.0000353	Pa×s	522.06	Joback Method
dvisc	0.0000184	Pa×s	551.29	Joback Method
dvisc	0.0000103	Pa×s	580.53	Joback Method
dvisc	0.0000060	Pa×s	609.76	Joback Method
dvisc	0.0000037	Pa×s	639.00	Joback Method
hvapt	84.90	kJ/mol	455.50	NIST Webbook

Sources

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=C533244&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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