

DIMETHYL 4-HYDROXYPTHALATE

Other names:	dimethyl 4-hydroxyphthalate
	Benzene-1,2-dicarboxylic acid, 4-hydroxy, dimethyl ester
Inchi:	InChI=1S/C10H10O5/c1-14-9(12)7-4-3-6(11)5-8(7)10(13)15-2/h3-5,11H,1-2H3
InchiKey:	JJXVDRYFBGDXOU-UHFFFAOYSA-N
Formula:	C10H10O5
SMILES:	COC(=O)c1ccc(O)cc1C(=O)OC
Mol. weight [g/mol]:	210.19

Physical Properties

Property code	Value	Unit	Source
af	0.7579		Cheméo Relay (1.0)
hf	-790.15	kJ/mol	Cheméo Relay (1.0)
hfus	26.67	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Cheméo Relay (1.0)
ie	8.89	eV	Cheméo Relay (1.0)
log10ws	-2.09		Cheméo Relay (1.0)
logp	0.965		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook
tb	580.03	K	Cheméo Relay (1.0)
tc	801.81	K	Cheméo Relay (1.0)
tf	375.27	K	Cheméo Relay (1.0)
vc	0.538	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.57	J/mol×K	693.06	Joback Method
cpg	437.01	J/mol×K	920.77	Joback Method
cpg	429.52	J/mol×K	882.82	Joback Method
cpg	421.52	J/mol×K	844.87	Joback Method
cpg	412.96	J/mol×K	806.92	Joback Method

cpg	403.80	J/mol×K	768.96	Joback Method
cpg	394.02	J/mol×K	731.01	Joback Method
dvisc	0.0000494	Pa×s	595.25	Joback Method
dvisc	0.0000171	Pa×s	693.06	Joback Method
dvisc	0.0000235	Pa×s	660.46	Joback Method
dvisc	0.0000334	Pa×s	627.85	Joback Method
dvisc	0.0002172	Pa×s	497.44	Joback Method
dvisc	0.0000764	Pa×s	562.65	Joback Method
dvisc	0.0001248	Pa×s	530.04	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22479954&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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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