

1,3-benzenedicarboxylic acid, 5-hydroxy-, dimethyl ester

Other names:	dimethyl 5-hydroxybenzene-1,3-dicarboxylate Benzene-1,3-dicarboxylic acid, 5-hydroxy, dimethyl ester
Inchi:	InChI=1S/C10H10O5/c1-14-9(12)6-3-7(10(13)15-2)5-8(11)4-6/h3-5,11H,1-2H3
InchiKey:	DOSDTCPDBPRFHQ-UHFFFAOYSA-N
Formula:	C10H10O5
SMILES:	<chem>COC(=O)c1cc(O)cc(C(=O)OC)c1</chem>
Mol. weight [g/mol]:	210.18

Physical Properties

Property code	Value	Unit	Source
gf	-486.36	kJ/mol	Joback Method
hf	-691.58	kJ/mol	Joback Method
hfus	26.67	kJ/mol	Joback Method
hvap	72.12	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.965		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
tb	693.06	K	Joback Method
tc	920.77	K	Joback Method
tf	497.44	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.57	J/molxK	693.06	Joback Method
cpg	394.02	J/molxK	731.01	Joback Method
cpg	403.80	J/molxK	768.96	Joback Method
cpg	412.96	J/molxK	806.92	Joback Method
cpg	421.52	J/molxK	844.87	Joback Method
cpg	429.52	J/molxK	882.82	Joback Method

cpg	437.01	J/mol×K	920.77	Joback Method
dvisc	0.0002172	Paxs	497.44	Joback Method
dvisc	0.0001248	Paxs	530.04	Joback Method
dvisc	0.0000764	Paxs	562.65	Joback Method
dvisc	0.0000494	Paxs	595.25	Joback Method
dvisc	0.0000334	Paxs	627.85	Joback Method
dvisc	0.0000235	Paxs	660.46	Joback Method
dvisc	0.0000171	Paxs	693.06	Joback Method

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=U400606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Crippen Method:	https://www.cheméo.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
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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