1,3-Benzenediol, monobenzoate

Other names:	Resorcinol, monobenzoate
	Benzoic acid, m-hydroxyphenyl ester
	Eastman Inhibitor RMB
	3-Hydroxyphenyl benzoate
	Benzoic acid resorcinol ester
	Resorcinol benzoate
Inchi:	InChI=1S/C13H10O3/c14-11-7-4-8-12(9-11)16-13(15)10-5-2-1-3-6-10/h1-9,14H
InchiKey:	GDESWOTWNNGOMW-UHFFFAOYSA-N
Formula:	C13H10O3
SMILES:	O=C(Oc1cccc(O)c1)c1ccccc1
Mol. weight [g/mol]:	214.22
CAS:	136-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-105.14	kJ/mol	Joback Method
hf	-260.70	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.611		Crippen Method
mcvol	159.820	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
tb	707.11	K	Joback Method
tc	962.79	K	Joback Method
tf	472.99	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.44	J/mol×K	707.11	Joback Method
cpg	425.94	J/mol×K	749.72	Joback Method
cpg	437.42	J/mol×K	792.34	Joback Method

cpg	448.02	J/mol×K	834.95	Joback Method
cpg	457.84	J/mol×K	877.56	Joback Method
cpg	467.02	J/mol×K	920.18	Joback Method
cpg	475.68	J/mol×K	962.79	Joback Method
dvisc	0.0003388	Pa×s	472.99	Joback Method
dvisc	0.0001645	Pa×s	512.01	Joback Method
dvisc	0.0000885	Pa×s	551.03	Joback Method
dvisc	0.0000517	Pa×s	590.05	Joback Method
dvisc	0.0000323	Pa×s	629.07	Joback Method
dvisc	0.0000213	Pa×s	668.09	Joback Method
dvisc	0.0000147	Pa×s	707.11	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C136367&Units=SI

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

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