1,3-Benzenediol, diacetate

Other names:	Resorcinol, diacetate
	m-Phenylenediacetate
	1,3-Diacetoxybenzene
	1,3-Dihydroxybenzene diacetate
	3-Phenylenediacetate
	Resorcinyl diacetate
	1,3-Benzenediol, 1,3-diacetate
	NSC 4885
	Dihydroxybenzene diacetate
	Resorcinyl acetate
	3-(Acetyloxy)phenyl acetate
Inchi:	InChI=1S/C10H10O4/c1-7(11)13-9-4-3-5-10(6-9)14-8(2)12/h3-6H,1-2H3
InchiKey:	STOUHHBZBQBYHH-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	CC(=O)Oc1cccc(OC(C)=O)c1
Mol. weight [g/mol]:	194.18
CAS:	108-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-331.74	kJ/mol	Joback Method
hf	-514.27	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	59.10	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.537		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
rinpol	1444.90		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1444.90		NIST Webbook
ripol	2301.00		NIST Webbook
ripol	2301.00		NIST Webbook
tb	551.00	K	NIST Webbook
tb	551.20	K	NIST Webbook
tc	831.50	K	Joback Method
tf	385.72	K	Joback Method

vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.80	J/mol×K	612.44	Joback Method
cpg	350.71	J/mol×K	648.95	Joback Method
cpg	361.93	J/mol×K	685.46	Joback Method
cpg	372.43	J/mol×K	721.97	Joback Method
cpg	382.23	J/mol×K	758.48	Joback Method
cpg	391.31	J/mol×K	794.99	Joback Method
cpg	399.66	J/mol×K	831.50	Joback Method
dvisc	0.0012091	Pa×s	385.72	Joback Method
dvisc	0.0007664	Pa×s	423.51	Joback Method
dvisc	0.0005235	Pa×s	461.29	Joback Method
dvisc	0.0003788	Pa×s	499.08	Joback Method
dvisc	0.0002869	Pa×s	536.87	Joback Method
dvisc	0.0002254	Pa×s	574.65	Joback Method
dvisc	0.0001824	Pa×s	612.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.20	K	1.60	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C108587&Units=SI

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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume