1,2,3-BENZENETRIYL ACETATE

Other names:	Acetpyrogall
	Lenigallol
	Pyracetol
	Pyrogallol triacetate
	Triacetylpyrogallol
	1,2,3-Triacetoxybenzene
	1,2,3-Phenenyl triacetate
	2,3-Bis(acetyloxy)phenyl acetate
	1,2,3-Benzenetriol, 1,2,3-triacetate
	NSC 24068
	benzene-1,2,3-triyl triacetate
Inchi:	InChI=1S/C12H12O6/c1-7(13)16-10-5-4-6-11(17-8(2)14)12(10)18-9(3)15/h4-6H,1-3H3
InchiKey:	AQGLTPNHAAVOKN-UHFFFAOYSA-N
Formula:	C12H12O6
SMILES:	CC(=O)Oc1cccc(OC(C)=O)c1OC(C)=O
Mol. weight [g/mol]:	252.22

Physical Properties

Property code	Value	Unit	Source
hf	-968.58	kJ/mol	Cheméo Relay (1.0)
hfus	28.46	kJ/mol	Joback Method
hvap	86.80	kJ/mol	Cheméo Relay (1.0)
ie	8.27	eV	Cheméo Relay (1.0)
log10ws	-2.19		Cheméo Relay (1.0)
logp	1.463		Crippen Method
mcvol	178.500	ml/mol	McGowan Method
tb	569.97	K	Cheméo Relay (1.0)
tf	339.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.46	J/mol×K	739.47	Joback Method
cpg	529.23	J/mol×K	956.11	Joback Method

cpg	522.27	J/mol×K	920.00	Joback Method
cpg	514.34	J/mol×K	883.89	Joback Method
cpg	505.47	J/mol×K	847.79	Joback Method
cpg	495.68	J/mol×K	811.68	Joback Method
cpg	485.01	J/mol×K	775.58	Joback Method
dvisc	0.0002275	Pa×s	616.21	Joback Method
dvisc	0.0001164	Pa×s	739.47	Joback Method
dvisc	0.0001418	Pa×s	698.38	Joback Method
dvisc	0.0001770	Pa×s	657.29	Joback Method
dvisc	0.0006214	Pa×s	492.94	Joback Method
dvisc	0.0003031	Pa×s	575.12	Joback Method
dvisc	0.0004222	Pa×s	534.03	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C525520&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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