

2,5-Diacetoxytoluene

Other names:	Methylhydroquinone, diacetate
Inchi:	InChI=1S/C11H12O4/c1-7-6-10(14-8(2)12)4-5-11(7)15-9(3)13/h4-6H,1-3H3
InchiKey:	KUZVIVNLNXNLAQ-UHFFFAOYSA-N
Formula:	C11H12O4
SMILES:	CC(=O)Oc1ccc(OC(C)=O)c(C)c1
Mol. weight [g/mol]:	208.21
CAS:	717-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-332.95	kJ/mol	Joback Method
hf	-546.38	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.846		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1523.10		NIST Webbook
tb	640.30	K	Joback Method
tc	856.49	K	Joback Method
tf	409.51	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.86	J/molxK	640.30	Joback Method
cpg	398.36	J/molxK	676.33	Joback Method
cpg	410.14	J/molxK	712.36	Joback Method
cpg	421.20	J/molxK	748.40	Joback Method
cpg	431.51	J/molxK	784.43	Joback Method
cpg	441.07	J/molxK	820.46	Joback Method
cpg	449.88	J/molxK	856.49	Joback Method

dvisc	0.0009633	Paxs	409.51	Joback Method
dvisc	0.0006315	Paxs	447.97	Joback Method
dvisc	0.0004426	Paxs	486.44	Joback Method
dvisc	0.0003268	Paxs	524.90	Joback Method
dvisc	0.0002515	Paxs	563.37	Joback Method
dvisc	0.0002001	Paxs	601.84	Joback Method
dvisc	0.0001637	Paxs	640.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C717271&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mvol:	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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