4-Acetoxy-2,5-dichlorophenyl acetate

Other names: 2,5-Dichlorobenzene-1,4-diol diacetate
Inchi: InChI=1S/C10H8Cl2O4/c1-5(13)15-9-3-8(12)10(4-7(9)11)16-6(2)14/h3-4H,1-2H3
InchiKey: QXTVIYNJMRUCPP-UHFFFAOYSA-N
Formula: C10H8Cl2O4
SMILES: CC(=O)Oc1cc(Cl)c(OC(C)=O)cc1Cl
Mol. weight [g/mol]: 263.07

Physical Properties

Property code	Value	Unit	Source
gf	-374.86	kJ/mol	Joback Method
hf	-568.69	kJ/mol	Joback Method
hfus	28.50	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.844		Crippen Method
mcvol	167.360	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
rinpol	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	697.26	K	Joback Method
tc	924.43	K	Joback Method
tf	470.60	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.86	J/mol×K	697.26	Joback Method
cpg	390.72	J/mol×K	735.12	Joback Method
cpg	399.88	J/mol×K	772.98	Joback Method
cpg	408.32	J/mol×K	810.85	Joback Method
cpg	416.03	J/mol×K	848.71	Joback Method
cpg	422.98	J/mol×K	886.57	Joback Method
cpg	429.17	J/mol×K	924.43	Joback Method

dvisc	0.0007277	Pa×s	470.60	Joback Method
dvisc	0.0005133	Pa×s	508.38	Joback Method
dvisc	0.0003800	Pa×s	546.15	Joback Method
dvisc	0.0002924	Pa×s	583.93	Joback Method
dvisc	0.0002323	Pa×s	621.71	Joback Method
dvisc	0.0001895	Pa×s	659.48	Joback Method
dvisc	0.0001580	Pa×s	697.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373208&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume