4-Allyl-1,2-diacetoxybenzene

Other names: 1,2-Diacetoxy-4-allylbenzene
Allylpyrocatechol diacetate
Inchi: InChI=1S/C13H14O4/c1-4-5-11-6-7-12(16-9(2)14)13(8-11)17-10(3)15/h4,6-8H,1,5H2,2-3
InchiKey: OLBAYJUQWFSQAY-UHFFFAOYSA-N
Formula: C13H14O4
SMILES: C=CCc1ccc(OC(C)=O)c(OC(C)=O)c1
Mol. weight [g/mol]: 234.25
CAS: 13620-82-1

Physical Properties

Property code	Value	Unit	Source
gf	-228.27	kJ/mol	Joback Method
hf	-462.23	kJ/mol	Joback Method
hfus	26.98	kJ/mol	Joback Method
hvap	65.77	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.266		Crippen Method
mcvol	180.850	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1638.20		NIST Webbook
rinpol	1638.20		NIST Webbook
tb	682.74	K	Joback Method
tc	895.98	K	Joback Method
tf	430.29	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.48	J/mol×K	682.74	Joback Method
cpg	476.61	J/mol×K	718.28	Joback Method
cpg	488.93	J/mol×K	753.82	Joback Method
cpg	500.43	J/mol×K	789.36	Joback Method

cpg	511.12	J/mol×K	824.90	Joback Method
cpg	520.99	J/mol×K	860.44	Joback Method
cpg	530.05	J/mol×K	895.98	Joback Method
dvisc	0.0008765	Pa×s	430.29	Joback Method
dvisc	0.0005632	Pa×s	472.37	Joback Method
dvisc	0.0003890	Pa×s	514.44	Joback Method
dvisc	0.0002842	Pa×s	556.51	Joback Method
dvisc	0.0002169	Pa×s	598.59	Joback Method
dvisc	0.0001716	Pa×s	640.66	Joback Method
dvisc	0.0001397	Pa×s	682.74	Joback Method

Sources

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=C13620821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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