

Allylpyrocatechol monoacetate

Inchi:	InChI=1S/C11H12O3/c1-3-4-9-5-6-11(10(13)7-9)14-8(2)12/h3,5-7,13H,1,4H2,2H3
InchiKey:	PNSJXUWAPPRSKA-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	<chem>C=CCc1ccc(OC(C)=O)c(O)c1</chem>
Mol. weight [g/mol]:	192.21

Physical Properties

Property code	Value	Unit	Source
gf	-156.18	kJ/mol	Joback Method
hf	-341.99	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	64.52	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.046		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
rinpol	1530.00		NIST Webbook
tb	636.33	K	Joback Method
tc	861.11	K	Joback Method
tf	434.79	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.79	J/molxK	636.33	Joback Method
cpg	428.53	J/molxK	823.65	Joback Method
cpg	419.24	J/molxK	786.18	Joback Method
cpg	409.38	J/molxK	748.72	Joback Method
cpg	398.90	J/molxK	711.26	Joback Method
cpg	387.72	J/molxK	673.79	Joback Method
cpg	437.33	J/molxK	861.11	Joback Method
dvisc	0.0000262	Paxs	636.33	Joback Method
dvisc	0.0000377	Paxs	602.74	Joback Method

dvisc	0.0000565	Paxs	569.15	Joback Method
dvisc	0.0000892	Paxs	535.56	Joback Method
dvisc	0.0001498	Paxs	501.97	Joback Method
dvisc	0.0002707	Paxs	468.38	Joback Method
dvisc	0.0005363	Paxs	434.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R441586&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

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