3-Acetoxy salicylic acid, phenyl ester

Inchi: InChI=1S/C15H12O5/c1-10(16)19-13-9-5-8-12(14(13)17)15(18)20-11-6-3-2-4-7-11/h2-9,
InchiKey: TVWZTHFHVCLXFL-UHFFFAOYSA-N
Formula: C15H12O5
SMILES: CC(=O)Oc1cccc(C(=O)Oc2ccccc2)c1O
Mol. weight [g/mol]: 272.25

Physical Properties

Property code	Value	Unit	Source
gf	-331.85	kJ/mol	Joback Method
hf	-558.25	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	85.52	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.537		Crippen Method
mcvol	195.440	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	834.14	K	Joback Method
tc	1080.69	K	Joback Method
tf	580.21	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.46	J/mol×K	834.14	Joback Method
cpg	560.90	J/mol×K	875.23	Joback Method
cpg	571.46	J/mol×K	916.32	Joback Method
cpg	581.21	J/mol×K	957.41	Joback Method
cpg	590.24	J/mol×K	998.50	Joback Method
cpg	598.64	J/mol×K	1039.59	Joback Method
cpg	606.48	J/mol×K	1080.69	Joback Method
dvisc	0.0000770	Pa×s	580.21	Joback Method
dvisc	0.0000429	Pa×s	622.53	Joback Method
dvisc	0.0000258	Pa×s	664.85	Joback Method

dvisc	0.0000165	Pa×s	707.17	Joback Method
dvisc	0.0000110	Pa×s	749.50	Joback Method
dvisc	0.0000077	Pa×s	791.82	Joback Method
dvisc	0.0000056	Pa×s	834.14	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=B6004194&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume