[1,1'-Binaphthalene]-3,3',4,4'-tetrol, tetra-acetate

Inchi: InChI=1S/C28H22O8/c1-15(29)33-25-13-23(19-9-5-7-11-21(19)27(25)35-17(3)31)24-14-

InchiKey: VTTKKLWKTBQZKA-UHFFFAOYSA-N

Formula: C28H22O8

SMILES: CC(=O)Oc1cc(-c2cc(OC(C)=O)c(OC(C)=O)c3ccccc23)c2ccccc2c1OC(C)=O

Mol. weight [g/mol]: 486.47

CAS: 7494-67-9

Physical Properties

Property code	Value	Unit	Source
gf	-370.46	kJ/mol	Joback Method
hf	-814.07	kJ/mol	Joback Method
hfus	59.21	kJ/mol	Joback Method
hvap	126.35	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	5.361		Crippen Method
mcvol	348.700	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
tb	1266.40	K	Joback Method
tc	1551.05	K	Joback Method
tf	887.32	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.97	J/mol×K	1266.40	Joback Method
cpg	1112.26	J/mol×K	1503.61	Joback Method
cpg	1115.67	J/mol×K	1456.17	Joback Method
cpg	1117.53	J/mol×K	1408.73	Joback Method
cpg	1117.76	J/mol×K	1361.28	Joback Method
cpg	1116.26	J/mol×K	1313.84	Joback Method
cpg	1107.39	J/mol×K	1551.05	Joback Method
dvisc	0.0000499	Pa×s	1266.40	Joback Method
dvisc	0.0000579	Pa×s	1203.22	Joback Method

dvisc	0.0000683	Pa×s	1140.04	Joback Method
dvisc	0.0000822	Pa×s	1076.86	Joback Method
dvisc	0.0001011	Pa×s	1013.68	Joback Method
dvisc	0.0001279	Pa×s	950.50	Joback Method
dvisc	0.0001673	Pa×s	887.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7494679&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
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume