Dihydroconiferyl benzoate

Inchi: InChI=1S/C17H18O4/c1-20-16-12-13(9-10-15(16)18)6-5-11-21-17(19)14-7-3-2-4-8-14/h2
InchiKey: PNPIRUVVJOWCSW-UHFFFAOYSA-N
Formula: C17H18O4
SMILES: COc1cc(CCCOC(=O)c2ccccc2)ccc1O
Mol. weight [g/mol]: 286.32
CAS: 147318-30-7

Physical Properties

Property code	Value	Unit	Source
gf	-186.09	kJ/mol	Joback Method
hf	-486.95	kJ/mol	Joback Method
hfus	37.24	kJ/mol	Joback Method
hvap	83.23	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.190		Crippen Method
mcvol	222.050	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	2424.10		NIST Webbook
rinpol	2424.10		NIST Webbook
tb	826.03	K	Joback Method
tc	1059.77	K	Joback Method
tf	552.82	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.50	J/mol×K	826.03	Joback Method
cpg	663.38	J/mol×K	864.99	Joback Method
cpg	676.32	J/mol×K	903.94	Joback Method
cpg	688.40	J/mol×K	942.90	Joback Method
cpg	699.70	J/mol×K	981.86	Joback Method
cpg	710.31	J/mol×K	1020.81	Joback Method
cpg	720.29	J/mol×K	1059.77	Joback Method

dvisc	0.0000872	Pa×s	552.82	Joback Method
dvisc	0.0000442	Pa×s	598.36	Joback Method
dvisc	0.0000247	Pa×s	643.89	Joback Method
dvisc	0.0000149	Pa×s	689.42	Joback Method
dvisc	0.0000096	Pa×s	734.96	Joback Method
dvisc	0.0000065	Pa×s	780.50	Joback Method
dvisc	0.0000046	Pa×s	826.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C147318307&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