1-Phenylcyclohexane-cis-1,2-diol-diacetate

Inchi: InChI=1S/C16H20O4/c1-12(17)19-15-10-6-7-11-16(15,20-13(2)18)14-8-4-3-5-9-14/h3-5,
InchiKey: SCUWPBGPZZKNHQ-UHFFFAOYSA-N
Formula: C16H20O4
SMILES: CC(=O)OC1CCCCC1(OC(C)=O)c1ccccc1
Mol. weight [g/mol]: 276.33
CAS: 23313-45-3

Physical Properties

Property code	Value	Unit	Source
chs	-8302.30	kJ/mol	NIST Webbook
gf	-260.34	kJ/mol	Joback Method
hf	-577.42	kJ/mol	Joback Method
hfus	23.42	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.951		Crippen Method
mcvol	216.560	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
tb	759.86	K	Joback Method
tc	996.52	K	Joback Method
tf	467.86	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.32	J/mol×K	759.86	Joback Method
cpg	659.68	J/mol×K	799.30	Joback Method
cpg	677.04	J/mol×K	838.75	Joback Method
cpg	693.53	J/mol×K	878.19	Joback Method
cpg	709.28	J/mol×K	917.63	Joback Method
cpg	724.42	J/mol×K	957.07	Joback Method
cpg	739.08	J/mol×K	996.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23313453&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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