(S)-2,3-dihydro-5-hydroxy-7-methoxy-2-phenyl-4-b

Other names: Pinostrobin
Inchi: InChI=1S/C16H14O4/c1-19-11-7-12(17)16-13(18)9-14(20-15(16)8-11)10-5-3-2-4-6-10/h2
InchiKey: ORJDDOBAOGKRJV-UHFFFAOYSA-N
Formula: C16H14O4
SMILES: COc1cc(O)c2c(c1)OC(c1ccccc1)CC2=O
Mol. weight [g/mol]: 270.28
CAS: 480-37-5

Physical Properties

Property code	Value	Unit	Source
gf	-130.28	kJ/mol	Joback Method
hf	-436.04	kJ/mol	Joback Method
hfus	34.99	kJ/mol	Joback Method
hvap	81.35	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.107		Crippen Method
mcvol	197.100	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	2434.20		NIST Webbook
rinpol	2434.20		NIST Webbook
tb	837.62	K	Joback Method
tc	1102.10	K	Joback Method
tf	591.12	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.69	J/mol×K	837.62	Joback Method
cpg	609.16	J/mol×K	881.70	Joback Method
cpg	622.52	J/mol×K	925.78	Joback Method
cpg	634.84	J/mol×K	969.86	Joback Method
cpg	646.26	J/mol×K	1013.94	Joback Method
cpg	656.86	J/mol×K	1058.02	Joback Method

cpg	666.76	J/mol×K	1102.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C480375&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
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