(S)-1,1-bis(4-Methoxyphenyl)propan-2-ol

Inchi: InChI=1S/C17H20O3/c1-12(18)17(13-4-8-15(19-2)9-5-13)14-6-10-16(20-3)11-7-14/h4-12
InchiKey: NHUSVJTYMHDUAP-LBPRGKRZSA-N
Formula: C17H20O3
SMILES: COc1ccc(C(c2ccc(OC)cc2)C(C)O)cc1
Mol. weight [g/mol]: 272.34
CAS: 212516-39-7

Physical Properties

Property code	Value	Unit	Source
gf	-53.88	kJ/mol	Joback Method
hf	-371.32	kJ/mol	Joback Method
hfus	26.51	kJ/mol	Joback Method
hvap	80.04	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.216		Crippen Method
mcvol	220.480	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	2276.50		NIST Webbook
rinpol	2276.50		NIST Webbook
tb	787.82	K	Joback Method
tc	1002.94	K	Joback Method
tf	434.51	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.91	J/mol×K	787.82	Joback Method
cpg	701.43	J/mol×K	967.08	Joback Method
cpg	691.18	J/mol×K	931.23	Joback Method
cpg	679.92	J/mol×K	895.38	Joback Method
cpg	667.64	J/mol×K	859.53	Joback Method
cpg	654.32	J/mol×K	823.67	Joback Method
cpg	710.71	J/mol×K	1002.94	Joback Method

dvisc	0.0000136	Pa×s	787.82	Joback Method
dvisc	0.0000203	Pa×s	728.93	Joback Method
dvisc	0.0000326	Pa×s	670.05	Joback Method
dvisc	0.0000572	Pa×s	611.16	Joback Method
dvisc	0.0001132	Pa×s	552.28	Joback Method
dvisc	0.0002638	Pa×s	493.39	Joback Method
dvisc	0.0007731	Pa×s	434.51	Joback Method

Sources

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=C212516397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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