1-(4-Methoxyphenyl)propane-1,2-diol

Inchi: InChI=1S/C10H14O3/c1-7(11)10(12)8-3-5-9(13-2)6-4-8/h3-7,10-12H,1-2H3
InchiKey: MRDZSBVJWOXBRW-UHFFFAOYSA-N
Formula: C10H14O3
SMILES: COc1ccc(C(O)C(C)O)cc1
Mol. weight [g/mol]: 182.22
CAS: 51410-48-1

Physical Properties

Property code	Value	Unit	Source
gf	-247.42	kJ/mol	Joback Method
hf	-471.91	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	75.78	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.109		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	1582.30		NIST Webbook
rinpol	1582.30		NIST Webbook
tb	665.76	K	Joback Method
tc	854.92	K	Joback Method
tf	355.27	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.88	J/mol×K	665.76	Joback Method
cpg	397.35	J/mol×K	697.29	Joback Method
cpg	407.25	J/mol×K	728.81	Joback Method
cpg	416.58	J/mol×K	760.34	Joback Method
cpg	425.37	J/mol×K	791.86	Joback Method
cpg	433.62	J/mol×K	823.39	Joback Method
cpg	441.35	J/mol×K	854.92	Joback Method

dvisc	0.0079564	Pa×s	355.27	Joback Method
dvisc	0.0013920	Pa×s	407.02	Joback Method
dvisc	0.0003609	Pa×s	458.77	Joback Method
dvisc	0.0001230	Pa×s	510.51	Joback Method
dvisc	0.0000511	Pa×s	562.26	Joback Method
dvisc	0.0000246	Pa×s	614.01	Joback Method
dvisc	0.0000133	Pa×s	665.76	Joback Method

Sources

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=C51410481&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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