1,3-Benzodioxol-4-ol, 2,2-dimethyl

Inchi: InChI=1S/C9H10O3/c1-9(2)11-7-5-3-4-6(10)8(7)12-9/h3-5,10H,1-2H3
InchiKey: CSSWBRMYHJVCPZ-UHFFFAOYSA-N
Formula: C9H10O3
SMILES: CC1(C)Oc2cccc(O)c2O1
Mol. weight [g/mol]: 166.17

Physical Properties

Property code	Value	Unit	Source
gf	-143.92	kJ/mol	Joback Method
hf	-357.30	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	59.36	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.899		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	1277.00		NIST Webbook
tb	578.48	K	Joback Method
tc	824.18	K	Joback Method
tf	436.83	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.17	J/mol×K	578.48	Joback Method
cpg	316.53	J/mol×K	619.43	Joback Method
cpg	326.96	J/mol×K	660.38	Joback Method
cpg	336.70	J/mol×K	701.33	Joback Method
cpg	346.01	J/mol×K	742.28	Joback Method
cpg	355.14	J/mol×K	783.23	Joback Method
cpg	364.34	J/mol×K	824.18	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=R84516&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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