1,4-benzodioxan-2-carboxylic acid

Inchi: InChI=1S/C9H8O4/c10-9(11)8-5-12-6-3-1-2-4-7(6)13-8/h1-4,8H,5H2,(H,10,11)
InchiKey: HMBHAQMOBKLWRX-UHFFFAOYSA-N
Formula: C9H8O4
SMILES: O=C(O)C1COc2ccccc2O1
Mol. weight [g/mol]: 180.16

Physical Properties

Property code	Value	Unit	Source
gf	-261.65	kJ/mol	Joback Method
hf	-466.20	kJ/mol	Joback Method
hfus	117.80	kJ/mol	Experimental and computational thermochemistry of 1,4-benzodioxan and its 2-R derivatives
hvap	71.10	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	0.911		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
pc	4602.62	kPa	Joback Method
tb	647.94	K	Joback Method
tc	869.24	K	Joback Method
tf	408.44	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.25	J/mol×K	647.94	Joback Method
cpg	329.48	J/mol×K	684.82	Joback Method
cpg	338.94	J/mol×K	721.71	Joback Method
cpg	347.69	J/mol×K	758.59	Joback Method
cpg	355.76	J/mol×K	795.47	Joback Method
cpg	363.20	J/mol×K	832.36	Joback Method
cpg	370.06	J/mol×K	869.24	Joback Method

dvisc	0.0028012	Pa×s	408.44	Joback Method
dvisc	0.0013773	Pa×s	448.36	Joback Method
dvisc	0.0007605	Pa×s	488.27	Joback Method
dvisc	0.0004594	Pa×s	528.19	Joback Method
dvisc	0.0002978	Pa×s	568.11	Joback Method
dvisc	0.0002044	Pa×s	608.02	Joback Method
dvisc	0.0001470	Pa×s	647.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemistry of 1,4-benzodioxan and its 2-R derivatives:	https://www.doi.org/10.1016/j.jct.2008.06.003
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume