1,3-Benzodioxole-5-carboxylic acid

Other names:	1,3-Benzodioxole-5-carboxylic acid (piperonylic acid) 3,4-methylenedioxybenzoic acid Heliotropic acid Protocatechuic acid methylene ether benzoic acid, 3,4-(methylenedioxy)- piperonylic acid protocatechuic acid methylen ether
Inchi:	InChI=1S/C8H6O4/c9-8(10)5-1-2-6-7(3-5)12-4-11-6/h1-3H,4H2,(H,9,10)
InchiKey:	VDVJGIYXDVPQLP-UHFFFAOYSA-N
Formula:	C8H6O4
SMILES:	O=C(O)c1ccc2c(c1)OCO2
Mol. weight [g/mol]:	166.13
CAS:	94-53-1

Physical Properties

Property code	Value	Unit	Source
gf	-259.89	kJ/mol	Joback Method
hf	-430.53	kJ/mol	Joback Method
hfus	28.45	kJ/mol	Joback Method
hsub	117.20 ± 1.80	kJ/mol	NIST Webbook
hvap	69.67	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.114		Crippen Method
mcvol	108.140	ml/mol	McGowan Method
pc	5213.15	kPa	Joback Method
tb	630.44	K	Joback Method
tc	849.52	K	Joback Method
tf	417.45	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.50	J/mol×K	849.52	Joback Method

cpg	267.00	J/mol×K	630.44	Joback Method
cpg	275.10	J/mol×K	666.95	Joback Method
cpg	282.59	J/mol×K	703.47	Joback Method
cpg	289.53	J/mol×K	739.98	Joback Method
cpg	295.96	J/mol×K	776.49	Joback Method
cpg	301.93	J/mol×K	813.01	Joback Method
dvisc	0.0001878	Pa×s	630.44	Joback Method
dvisc	0.0023959	Pa×s	417.45	Joback Method
dvisc	0.0013273	Pa×s	452.95	Joback Method
dvisc	0.0008012	Pa×s	488.45	Joback Method
dvisc	0.0005179	Pa×s	523.95	Joback Method
dvisc	0.0003538	Pa×s	559.44	Joback Method
dvisc	0.0002529	Pa×s	594.94	Joback Method
hfust	30.50	kJ/mol	501.60	NIST Webbook
hsubt	113.60 ± 1.10	kJ/mol	370.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Construction, calibration and testing of a micro-combustion calorimeter: https://www.doi.org/10.1016/j.jct.2006.03.001

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=C94531&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
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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