

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
mvol	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	m ³ /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	Paxs	630.44	Joback Method
dvisc	0.0023959	Paxs	417.45	Joback Method
dvisc	0.0013273	Paxs	452.95	Joback Method
dvisc	0.0008012	Paxs	488.45	Joback Method
dvisc	0.0005179	Paxs	523.95	Joback Method
dvisc	0.0003538	Paxs	559.44	Joback Method
dvisc	0.0002529	Paxs	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

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/ci990307i
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

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

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