3,4-Methylenedioxyphenylacetic acid

Other names:	1,3-Benzodioxole-5-acetic acid
	Homopiperonylic acid
	benzo-1,3-dioxole-5-acetic acid
	1,3-Benzodioxole-5-acetic acid (homopiperonylic acid)
Inchi:	InChI=1S/C9H8O4/c10-9(11)4-6-1-2-7-8(3-6)13-5-12-7/h1-3H,4-5H2,(H,10,11)
InchiKey:	ODVLMCWNGKLROU-UHFFFAOYSA-N
Formula:	C9H8O4
SMILES:	O=C(O)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	180.16
CAS:	2861-28-1

Physical Properties

Property code	Value	Unit	Source
gf	-251.47	kJ/mol	Joback Method
hf	-451.17	kJ/mol	Joback Method
hfus	31.04	kJ/mol	Joback Method
hsub	122.90 ± 1.40	kJ/mol	NIST Webbook
hvap	71.89	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.042		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	653.32	K	Joback Method
tc	868.68	K	Joback Method
tf	428.72	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.65	J/mol×K	868.68	Joback Method
cpg	313.40	J/mol×K	653.32	Joback Method
cpg	322.35	J/mol×K	689.21	Joback Method
cpg	330.67	J/mol×K	725.11	Joback Method

cpg	338.41	J/mol×K	761.00	Joback Method
cpg	345.62	J/mol×K	796.89	Joback Method
cpg	352.35	J/mol×K	832.78	Joback Method
dvisc	0.0001619	Pa×s	653.32	Joback Method
dvisc	0.0021756	Pa×s	428.72	Joback Method
dvisc	0.0011858	Pa×s	466.15	Joback Method
dvisc	0.0007073	Pa×s	503.59	Joback Method
dvisc	0.0004532	Pa×s	541.02	Joback Method
dvisc	0.0003076	Pa×s	578.45	Joback Method
dvisc	0.0002188	Pa×s	615.89	Joback Method
hfust	24.94	kJ/mol	401.70	NIST Webbook
hsubt	120.10 ± 0.80	kJ/mol	355.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2861281&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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