

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	m ³ /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	Paxs	653.32	Joback Method
dvisc	0.0021756	Paxs	428.72	Joback Method
dvisc	0.0011858	Paxs	466.15	Joback Method
dvisc	0.0007073	Paxs	503.59	Joback Method
dvisc	0.0004532	Paxs	541.02	Joback Method
dvisc	0.0003076	Paxs	578.45	Joback Method
dvisc	0.0002188	Paxs	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

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=C2861281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	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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