3-(3,4-Methylendioxyphenyl)propionic acid

Other names: 1,3-Benzodioxole-5-propanoic acid
3,4-(Methylenedioxy)hydrocinnamic acid
3-(3,4-Methylenedioxyphenyl)propionic acid
Hydrocinnamic acid, 3,4-(methylenedioxy)-
benzo-1,3-dioxole-5-propionic acid
Inchi: InChI=1S/C10H10O4/c11-10(12)4-2-7-1-3-8-9(5-7)14-6-13-8/h1,3,5H,2,4,6H2,(H,11,12)
InchiKey: UIYJGLLTSVRSBM-UHFFFAOYSA-N
Formula: C10H10O4
SMILES: O=C(O)CCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 194.19

Physical Properties

Property code	Value	Unit	Source
hfus	33.63	kJ/mol	Joback Method
hvap	101.88	kJ/mol	Cheméo Relay (1.0)
ie	8.22	eV	Cheméo Relay (1.0)
log10ws	-2.33		Cheméo Relay (1.0)
logp	1.432		Crippen Method
mcvol	136.320	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	588.25	K	Cheméo Relay (1.0)
tf	372.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.32	J/mol×K	676.20	Joback Method
cpg	371.03	J/mol×K	711.53	Joback Method
cpg	380.09	J/mol×K	746.85	Joback Method
cpg	388.54	J/mol×K	782.18	Joback Method
cpg	396.44	J/mol×K	817.51	Joback Method
cpg	403.84	J/mol×K	852.84	Joback Method
cpg	410.80	J/mol×K	888.16	Joback Method
dvisc	0.0019615	Pa×s	439.99	Joback Method

dvisc	0.0010527	Pa×s	479.36	Joback Method
dvisc	0.0006209	Pa×s	518.73	Joback Method
dvisc	0.0003946	Pa×s	558.10	Joback Method
dvisc	0.0002662	Pa×s	597.46	Joback Method
dvisc	0.0001885	Pa×s	636.83	Joback Method
dvisc	0.0001390	Pa×s	676.20	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2815954&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point