

3-(3-Hydroxyphenyl)propionic acid

Other names:	«beta»-(m-Hydroxyphenyl)propionic acid Benzenepropanoic acid, 3-hydroxy- «beta»-(3-Hydroxyphenyl)propionic acid m-Hydroxyphenylpropionic acid Hydrocinnamic acid, m-hydroxy- 3-(m-Hydroxyphenyl)propionic acid 3-Hydroxyphenylpropionic acid 3-Hydroxybenzenepropanoic acid Dihydro-m-coumaric acid NSC 33135 NSC 39468
Inchi:	InChI=1S/C9H10O3/c10-8-3-1-2-7(6-8)4-5-9(11)12/h1-3,6,10H,4-5H2,(H,11,12)
InchiKey:	QVWAEZJXDYOKEH-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	O=C(O)CCc1cccc(O)c1
Mol. weight [g/mol]:	166.17
CAS:	621-54-5

Physical Properties

Property code	Value	Unit	Source
gf	-283.05	kJ/mol	Joback Method
hf	-434.68	kJ/mol	Joback Method
hfus	24.58	kJ/mol	Joback Method
hvap	74.34	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.409		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
tb	658.67	K	Joback Method
tc	871.60	K	Joback Method
tf	440.08	K	Joback Method
vc	0.422	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.04	J/molxK	658.67	Joback Method
cpg	334.12	J/molxK	694.16	Joback Method
cpg	342.62	J/molxK	729.65	Joback Method
cpg	350.59	J/molxK	765.14	Joback Method
cpg	358.12	J/molxK	800.63	Joback Method
cpg	365.26	J/molxK	836.12	Joback Method
cpg	372.09	J/molxK	871.60	Joback Method
dvisc	0.0006700	Paxs	440.08	Joback Method
dvisc	0.0002502	Paxs	476.51	Joback Method
dvisc	0.0001075	Paxs	512.94	Joback Method
dvisc	0.0000516	Paxs	549.38	Joback Method
dvisc	0.0000272	Paxs	585.81	Joback Method
dvisc	0.0000154	Paxs	622.24	Joback Method
dvisc	0.0000093	Paxs	658.67	Joback Method

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=C621545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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