Mandelic acid

Other names:

(+)-(S)-mandelic acid
(+)-mandelic acid
(.+/-.)-Mandelic acid
(.+/-.)-alpha-Hydroxybenzeneacetic acid
(RS)-Mandelic acid
(S)-(+)-mandelic acid
(S)-.alpha.-hydroxybenzeneacetic acid
(S)-2-hydroxy-2-phenylacetic acid
(S)-mandelic acid
114-21-6
2-Phenyl-2-hydroxyacetic acid
2-Phenylglycolic acid
530-31-4
Almond acid
Amygdalic acid
Amygdalinic acid
Benzeneacetic acid, «alpha»-hydroxy-
Benzeneacetic acid, «alpha»-hydroxy-, (.+/-.)-
Benzoglycolic acid
DL-Hydroxy(phenyl)acetic acid
Glycolic acid, phenyl-
Hydroxy(phenyl)acetic acid
Kyselina 2-fenyl-2-hydroxyethanova
Kyselina mandlova
L-(+)-mandelate
L-(+)-mandelic acid
L-mandelic acid
NSC 7925
Paramandelic acid
Phenylglycolic acid
Phenylhydroxyacetic acid
Racemic mandelic acid
S-(+)-mandelic acid
Uromaline
benzeneacetic acid, .alpha.-hydroxy-, (S)-
dl-Mandelic acid
ethanoic acid, 2-hydroxy-2-phenyl-, (S)-
mandelic acid, L-(+)-
p-Mandelic acid
«alpha»-Hydroxy-«alpha»-toluic acid

«alpha»-Hydroxyphenylacetic acid
«alpha»-Phenylhydroxyacetic acid
«alpha»-Toluic acid, «alpha»-hydroxy-

Inchi: InChI=1S/C8H8O3/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7,9H,(H,10,11)
InchiKey: IWYDHOAUDWTVEP-UHFFFAOYSA-N
Formula: C8H8O3
SMILES: O=C(O)C(O)c1ccccc1
Mol. weight [g/mol]: 152.15
CAS: 611-72-3

Physical Properties

Property code	Value	Unit	Source
chs	-3712.00 ± 0.80	kJ/mol	NIST Webbook
gf	-276.11	kJ/mol	Joback Method
hf	-394.24	kJ/mol	Joback Method
hfus	16.77	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	0.805		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	5102.04	kPa	Joback Method
tb	646.91	K	Joback Method
tc	844.13	K	Joback Method
tf	407.70	K	Experimental and theoretical thermodynamic properties of RS-(+-)- and S-(+)-mandelic acids
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.92	J/mol×K	646.91	Joback Method
cpg	286.85	J/mol×K	679.78	Joback Method
cpg	294.26	J/mol×K	712.65	Joback Method
cpg	301.16	J/mol×K	745.52	Joback Method
cpg	307.59	J/mol×K	778.39	Joback Method
cpg	313.57	J/mol×K	811.26	Joback Method

cpg	319.12	J/mol×K	844.13	Joback Method
dvisc	0.0084829	Pa×s	362.91	Joback Method
dvisc	0.0018322	Pa×s	410.24	Joback Method
dvisc	0.0005434	Pa×s	457.58	Joback Method
dvisc	0.0002024	Pa×s	504.91	Joback Method
dvisc	0.0000893	Pa×s	552.24	Joback Method
dvisc	0.0000448	Pa×s	599.58	Joback Method
dvisc	0.0000249	Pa×s	646.91	Joback Method

Sources

Experimental and theoretical thermodynamic properties of RS-(+-)- and S-(+)-mandelic acids:	https://www.doi.org/10.1016/j.tca.2018.05.010
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=C611723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
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