Mandelic acid

Other names:	Benzeneacetic acid, «alpha»-hydroxy-
	«alpha»-Hydroxy-«alpha»-toluic acid
	«alpha»-Hydroxyphenylacetic acid
	p-Mandelic acid
	Almond acid
	Amygdalic acid
	Amygdalinic acid
	Phenylglycolic acid
	Phenylhydroxyacetic acid
	Uromaline
	dl-Mandelic acid
	«alpha»-Toluic acid, «alpha»-hydroxy-
	Glycolic acid, phenyl-
	Racemic mandelic acid
	Kyselina 2-fenyl-2-hydroxyethanova
	Kyselina mandlova
	Paramandelic acid
	«alpha»-Phenylhydroxyacetic acid
	Benzoglycolic acid
	Hydroxy(phenyl)acetic acid
	Benzeneacetic acid, «alpha»-hydroxy-, (.+/-.)-
	(.+/-.)-alpha-Hydroxybenzeneacetic acid
	(.+/-.)-Mandelic acid
	(RS)-Mandelic acid
	2-Phenyl-2-hydroxyacetic acid
	2-Phenylglycolic acid
	DL-Hydroxy(phenyl)acetic acid
	NSC 7925
	114-21-6
	530-31-4
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:	90-64-2

Physical Properties

Property code	Value	Unit	Source
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
rinpol	1487.00		NIST Webbook
tb	646.91	K	Joback Method
tc	844.13	K	Joback Method
tf	392.00 ± 1.50	K	NIST Webbook
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.57	J/mol×K	811.26	Joback Method
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	319.12	J/mol×K	844.13	Joback Method
cps	199.20	J/mol×K	323.00	NIST Webbook
dvisc	0.0000249	Pa×s	646.91	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
hfust	25.52	kJ/mol	392.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90642&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume