

# 2,6-Difluoromandelic acid

<b>Inchi:</b>	InChI=1S/C8H6F2O3/c9-4-2-1-3-5(10)6(4)7(11)8(12)13/h1-3,7,11H,(H,12,13)
<b>InchiKey:</b>	BMZWDQNFSCPCFG-UHFFFAOYSA-N
<b>Formula:</b>	C8H6F2O3
<b>SMILES:</b>	O=C(O)C(O)c1c(F)cccc1F
<b>Mol. weight [g/mol]:</b>	188.13
<b>CAS:</b>	207981-50-8

## Physical Properties

Property code	Value	Unit	Source
gf	-684.99	kJ/mol	Joback Method
hf	-809.40	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	75.08	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.083		Crippen Method
mcvol	116.670	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
tb	655.41	K	Joback Method
tc	839.59	K	Joback Method
tf	389.13	K	Joback Method
vc	0.450	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.91	J/molxK	655.41	Joback Method
cpg	298.85	J/molxK	686.11	Joback Method
cpg	305.38	J/molxK	716.80	Joback Method
cpg	311.50	J/molxK	747.50	Joback Method
cpg	317.24	J/molxK	778.20	Joback Method
cpg	322.60	J/molxK	808.89	Joback Method
cpg	327.61	J/molxK	839.59	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C207981508&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C207981508&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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