

Mandelic acid, alpha-cyclopentyl

Other names:	cyclopentylphenylglycolic acid
Inchi:	InChI=1S/C13H16O3/c14-12(15)13(16,11-8-4-5-9-11)10-6-2-1-3-7-10/h1-3,6-7,11,16H,4
InchiKey:	WFLUEQCOAQCQLP-UHFFFAOYSA-N
Formula:	C13H16O3
SMILES:	O=C(O)C(O)(c1ccccc1)C1CCCC1
Mol. weight [g/mol]:	220.26
CAS:	427-49-6

Physical Properties

Property code	Value	Unit	Source
gf	-192.18	kJ/mol	Joback Method
hf	-440.43	kJ/mol	Joback Method
hfus	19.76	kJ/mol	Joback Method
hvap	85.87	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.149		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	773.80	K	Joback Method
tc	987.44	K	Joback Method
tf	447.58	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.46	J/molxK	773.80	Joback Method
cpg	571.63	J/molxK	951.83	Joback Method
cpg	562.85	J/molxK	916.22	Joback Method
cpg	553.42	J/molxK	880.62	Joback Method
cpg	543.27	J/molxK	845.01	Joback Method
cpg	532.31	J/molxK	809.41	Joback Method
cpg	579.84	J/molxK	987.44	Joback Method
dvisc	0.0000099	Paxs	773.80	Joback Method

dvisc	0.0000169	Paxs	719.43	Joback Method
dvisc	0.0000312	Paxs	665.06	Joback Method
dvisc	0.0000642	Paxs	610.69	Joback Method
dvisc	0.0001526	Paxs	556.32	Joback Method
dvisc	0.0004370	Paxs	501.95	Joback Method
dvisc	0.0016162	Paxs	447.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=C427496&Units=SI

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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