4-Fluoromandelic acid

Other names: Benzeneacetic acid, 4-fluoro-«alpha»-hydroxy-
(dl) p-fluoromandelic acid
Inchi: InChI=1S/C8H7FO3/c9-6-3-1-5(2-4-6)7(10)8(11)12/h1-4,7,10H,(H,11,12)
InchiKey: RWCMOQXHIDWDDJ-UHFFFAOYSA-N
Formula: C8H7FO3
SMILES: O=C(O)C(O)c1ccc(F)cc1
Mol. weight [g/mol]: 170.14
CAS: 395-33-5

Physical Properties

Property code	Value	Unit	Source
gf	-480.55	kJ/mol	Joback Method
hf	-601.82	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	75.24	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	0.944		Crippen Method
mcvol	114.900	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
tb	651.16	K	Joback Method
tc	841.52	K	Joback Method
tf	376.02	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.45	J/mol×K	651.16	Joback Method
cpg	292.86	J/mol×K	682.89	Joback Method
cpg	299.80	J/mol×K	714.61	Joback Method
cpg	306.30	J/mol×K	746.34	Joback Method
cpg	312.37	J/mol×K	778.07	Joback Method
cpg	318.03	J/mol×K	809.79	Joback Method
cpg	323.30	J/mol×K	841.52	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=C395335&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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