

BENZENEACETIC ACID, 4-FLUORO-.ALPHA.-HYDROXY-

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

Physical Properties

Property code	Value	Unit	Source
hfus	19.46	kJ/mol	Joback Method
ie	9.12	eV	Cheméo Relay (1.0)
log10ws	-0.43		Cheméo Relay (1.0)
logp	0.944		Crippen Method
mcvol	114.900	ml/mol	McGowan Method
tf	404.57	K	Cheméo Relay (1.0)

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
hfust	29.29	kJ/mol	403.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C395335&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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