

4-Fluoroveratrole

Other names:	Fluorobenzene, 3,4-methoxy- 4-Fluoro-2-methoxyphenol, methyl ether 4-Fluoro-1,2-dimethoxybenzene
Inchi:	InChI=1S/C8H9FO2/c1-10-7-4-3-6(9)5-8(7)11-2/h3-5H,1-2H3
InchiKey:	DAGKHJDZYJFWSO-UHFFFAOYSA-N
Formula:	C8H9FO2
SMILES:	COc1ccc(F)cc1OC
Mol. weight [g/mol]:	156.15
CAS:	398-62-9

Physical Properties

Property code	Value	Unit	Source
gf	-295.18	kJ/mol	Joback Method
hf	-455.41	kJ/mol	Joback Method
hfus	15.20	kJ/mol	Joback Method
hvap	41.00	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.843		Crippen Method
mcvol	113.330	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1157.40		NIST Webbook
tb	463.19	K	Joback Method
tc	661.91	K	Joback Method
tf	276.43	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.97	J/mol×K	463.19	Joback Method
cpg	240.64	J/mol×K	496.31	Joback Method
cpg	250.93	J/mol×K	529.43	Joback Method
cpg	260.85	J/mol×K	562.55	Joback Method
cpg	270.37	J/mol×K	595.67	Joback Method

cpg	279.49	J/mol×K	628.79	Joback Method
cpg	288.21	J/mol×K	661.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C398629&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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