

BENZENE

1,2,4,5-TETRAFLUORO-3,6-DIMETHOXY-

Other names:	Tetrafluorohydroquinone, dimethyl ether 1,2,4,5-Tetrafluoro-3,6-dimethoxybenzene
Inchi:	InChI=1S/C8H6F4O2/c1-13-7-3(9)5(11)8(14-2)6(12)4(7)10/h1-2H3
InchiKey:	WQXKGOOORHDGFP-UHFFFAOYSA-N
Formula:	C8H6F4O2
SMILES:	COc1c(F)c(F)c(OC)c(F)c1F
Mol. weight [g/mol]:	210.13

Physical Properties

Property code	Value	Unit	Source
hfus	23.27	kJ/mol	Joback Method
ie	8.77	eV	Cheméo Relay (1.0)
logp	2.260		Crippen Method
mcvol	118.640	ml/mol	McGowan Method
rinpol	1069.80		NIST Webbook
tb	446.57	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.36	J/mol×K	475.94	Joback Method
cpg	263.54	J/mol×K	504.92	Joback Method
cpg	271.55	J/mol×K	533.90	Joback Method
cpg	279.37	J/mol×K	562.88	Joback Method
cpg	286.98	J/mol×K	591.86	Joback Method
cpg	294.37	J/mol×K	620.84	Joback Method
cpg	301.52	J/mol×K	649.82	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C362561&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/ci990307I>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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