

Benzene, pentachloro, ethoxy-

Other names:	Benzene, pentachloro, ethoxy-
Inchi:	InChI=1S/C8H5Cl5O/c1-2-14-8-6(12)4(10)3(9)5(11)7(8)13/h2H2,1H3
InchiKey:	YXNDWTIYDLVODL-UHFFFAOYSA-N
Formula:	C8H5Cl5O
SMILES:	CCOc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	294.39

Physical Properties

Property code	Value	Unit	Source
hf	-191.15	kJ/mol	Cheméo Relay (1.0)
hfus	30.75	kJ/mol	Joback Method
hvap	77.18	kJ/mol	Cheméo Relay (1.0)
ie	8.51	eV	Cheméo Relay (1.0)
log10ws	-6.43		Cheméo Relay (1.0)
logp	5.352		Crippen Method
mcvol	166.890	ml/mol	McGowan Method
tb	578.05	K	Cheméo Relay (1.0)
tf	390.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.34	J/mol×K	643.59	Joback Method
cpg	314.07	J/mol×K	683.24	Joback Method
cpg	321.32	J/mol×K	722.88	Joback Method
cpg	328.10	J/mol×K	762.53	Joback Method
cpg	334.40	J/mol×K	802.17	Joback Method
cpg	340.19	J/mol×K	841.82	Joback Method
cpg	345.48	J/mol×K	881.47	Joback Method
dvisc	0.0006816	Pa×s	440.77	Joback Method
dvisc	0.0005080	Pa×s	474.57	Joback Method
dvisc	0.0003937	Pa×s	508.38	Joback Method
dvisc	0.0003149	Pa×s	542.18	Joback Method
dvisc	0.0002586	Pa×s	575.98	Joback Method

dvisc	0.0002171	Pa×s	609.79	Joback Method
dvisc	0.0001856	Pa×s	643.59	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10463102&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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