Benzene, 2,4,6-trichloro-1-ethoxy

Other names:	Ethyl 2,4,6-trichlorophenyl ether
	Benzene, 1-ethoxy-2,4,6-trichloro
	Benzene, 1,3,5-trichloro-2-ethoxy-
	2,4,6-trichlorophenetole
Inchi:	InChI=1S/C8H7Cl3O/c1-2-12-8-6(10)3-5(9)4-7(8)11/h3-4H,2H2,1H3
InchiKey:	GYDFVBYBCDOBFE-UHFFFAOYSA-N
Formula:	C8H7Cl3O
SMILES:	CCOc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	225.50
CAS:	23399-88-4

Physical Properties

Property code	Value	Unit	Source
gf	-40.79	kJ/mol	Joback Method
hf	-185.77	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	53.23	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	4.045		Crippen Method
mcvol	142.410	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	1406.00		NIST Webbook
tb	558.77	K	Joback Method
tc	787.57	K	Joback Method
tf	355.89	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.21	J/mol×K	558.77	Joback Method
cpg	311.52	J/mol×K	749.44	Joback Method
cpg	304.09	J/mol×K	711.30	Joback Method
cpg	296.15	J/mol×K	673.17	Joback Method

cpg	287.69	J/mol×K	635.04	Joback Method
cpg	278.71	J/mol×K	596.90	Joback Method
cpg	318.44	J/mol×K	787.57	Joback Method
dvisc	0.0002120	Pa×s	558.77	Joback Method
dvisc	0.0002543	Pa×s	524.96	Joback Method
dvisc	0.0003128	Pa×s	491.14	Joback Method
dvisc	0.0003968	Pa×s	457.33	Joback Method
dvisc	0.0005228	Pa×s	423.52	Joback Method
dvisc	0.0007225	Pa×s	389.70	Joback Method
dvisc	0.0010618	Pa×s	355.89	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23399884&Units=SI
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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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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