Benzenemethanol, 2-chloro-«alpha»-(4-chlorophenyl)-«alpha»-(trichl

Other names: Benzenemethanol, 4-chloro-«alpha»-(2-chlorophenyl)-«alpha»-(trichloromethyl)-
o,p-Dicofol
Ethanol, 1-(2-chlorophenyl)-1-(4-chlorophenyl)-2,2,2-trichloro-
2-Chloro-«alpha»-(4-chlorophenyl)-«alpha»-(trichloromethyl)benzenemethanol

Inchi: InChI=1S/C14H9Cl5O/c15-10-7-5-9(6-8-10)13(20,14(17,18)19)11-3-1-2-4-12(11)16/h1-8

InchiKey: LUXSISXJGNCOKN-UHFFFAOYSA-N

Formula: C14H9Cl5O

SMILES: OC(c1ccc(Cl)cc1)(c1ccccc1Cl)C(Cl)(Cl)Cl

Mol. weight [g/mol]: 370.49

CAS: 10606-46-9

Physical Properties

Property code	Value	Unit	Source
gf	81.77	kJ/mol	Joback Method
hf	-130.60	kJ/mol	Joback Method
hfus	29.57	kJ/mol	Joback Method
hvap	88.65	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.599		Crippen Method
mcvol	227.670	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
tb	855.91	K	Joback Method
tc	1113.69	K	Joback Method
tf	397.07 ± 0.20	K	NIST Webbook
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.02	J/mol×K	855.91	Joback Method
cpg	544.31	J/mol×K	898.87	Joback Method
cpg	551.91	J/mol×K	941.84	Joback Method
cpg	559.01	J/mol×K	984.80	Joback Method
cpg	565.76	J/mol×K	1027.76	Joback Method

cpg	572.34	J/mol×K	1070.72	Joback Method
cpg	578.92	J/mol×K	1113.69	Joback Method
dvisc	0.0002838	Pa×s	540.68	Joback Method
dvisc	0.0001325	Pa×s	593.22	Joback Method
dvisc	0.0000700	Pa×s	645.76	Joback Method
dvisc	0.0000407	Pa×s	698.30	Joback Method
dvisc	0.0000256	Pa×s	750.83	Joback Method
dvisc	0.0000170	Pa×s	803.37	Joback Method
dvisc	0.0000119	Pa×s	855.91	Joback Method
hfust	25.20	kJ/mol	396.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10606469&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hfust: Enthalpy of fusion at a given temperature
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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