2,2,2-Trichloro-1-phenylethanol

Other names:	Benzenemethanol, «alpha»-(trichloromethyl)- «alpha»-(Trichloromethyl)benzyl alcohol Benzyl alcohol, «alpha»-(trichloromethyl)- Efiran 99 Phenyl(trichloromethyl)carbinol 1-Phenyl-2,2,2-trichloroethanol «alpha»-(Trichloromethyl)benzenemethanol Trichloromethylphenyl carbinol NSC 2796
Inchi:	InChI=1S/C8H7Cl3O/c9-8(10,11)7(12)6-4-2-1-3-5-6/h1-5,7,12H
InchiKey:	ABFRBTDJEKZSRM-UHFFFAOYSA-N
Formula:	C8H7Cl3O
SMILES:	OC(c1ccccc1)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	225.50
CAS:	2000-43-3

Physical Properties

Property code	Value	Unit	Source
gf	-43.32	kJ/mol	Joback Method
hf	-185.40	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	63.83	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.090		Crippen Method
mcvol	142.410	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	609.92	K	Joback Method
tc	838.14	K	Joback Method
tf	344.34	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	296.33	J/mol×K	609.92	Joback Method
cpg	305.36	J/mol×K	647.96	Joback Method
cpg	313.56	J/mol×K	685.99	Joback Method
cpg	321.00	J/mol×K	724.03	Joback Method
cpg	327.76	J/mol×K	762.07	Joback Method
cpg	333.91	J/mol×K	800.11	Joback Method
cpg	339.52	J/mol×K	838.14	Joback Method
dvisc	0.0074050	Pa×s	344.34	Joback Method
dvisc	0.0022441	Pa×s	388.60	Joback Method
dvisc	0.0008682	Pa×s	432.87	Joback Method
dvisc	0.0004006	Pa×s	477.13	Joback Method
dvisc	0.0002108	Pa×s	521.39	Joback Method
dvisc	0.0001226	Pa×s	565.66	Joback Method
dvisc	0.0000772	Pa×s	609.92	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2000433&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
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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