1,1-Bis-(4-bromophenyl)-2,2,2-trichloroethane

Other names: Benzene, 1,1'-(2,2,2-trichloroethylidene)bis(4-bromo-
Ethane, 2,2-bis(p-bromophenyl)-1,1,1-trichloro-
Ethane, 2,2-bis(4-bromophenyl)-1,1,1-trichloro-
1,1-Bis(p-bromophenyl)-2,2,2-trichloroethane
1,1,1-Trichloro-2,2-bis(p-bromophenyl)ethane
2,2-Bis(p-bromophenyl)-1,1,1-trichloroethane
2,2-Bis(4-bromophenyl)-1,1,1-trichloroethane
1,1-Bis-(4-bromophenyl)-2,2,2-trichloroethane
NSC 2367

Inchi: InChI=1S/C14H9Br2Cl3/c15-11-5-1-9(2-6-11)13(14(17,18)19)10-3-7-12(16)8-4-10/h1-8,1

InchiKey: YPWDDFGPYBIPBG-UHFFFAOYSA-N

Formula: C14H9Br2Cl3

SMILES: ClC(Cl)(Cl)C(c1ccc(Br)cc1)c1ccc(Br)cc1

Mol. weight [g/mol]: 443.39

Physical Properties

Property code	Value	Unit	Source
hfus	31.54	kJ/mol	Joback Method
ie	8.72	eV	Cheméo Relay (1.0)
log10ws	-7.91		Cheméo Relay (1.0)
logp	6.714		Crippen Method
mcvol	232.320	ml/mol	McGowan Method
tb	661.15	K	Cheméo Relay (1.0)
tf	391.10	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.31	J/mol×K	823.98	Joback Method
cpg	520.50	J/mol×K	872.42	Joback Method
cpg	529.75	J/mol×K	920.86	Joback Method
cpg	538.29	J/mol×K	969.30	Joback Method
cpg	546.33	J/mol×K	1017.74	Joback Method
cpg	554.10	J/mol×K	1066.18	Joback Method

cpg	561.82	J/mol×K	1114.63	Joback Method
dvisc	0.0005867	Pa×s	522.20	Joback Method
dvisc	0.0003569	Pa×s	572.50	Joback Method
dvisc	0.0002352	Pa×s	622.79	Joback Method
dvisc	0.0001650	Pa×s	673.09	Joback Method
dvisc	0.0001216	Pa×s	723.39	Joback Method
dvisc	0.0000932	Pa×s	773.68	Joback Method
dvisc	0.0000739	Pa×s	823.98	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2990172&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/ci990307l

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

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion 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