

Ethane, 2-(p-bromophenyl)-1,1,1-trichloro-2-phenyl-

Inchi: InChI=1S/C14H10BrCl3/c15-12-8-6-11(7-9-12)13(14(16,17)18)10-4-2-1-3-5-10/h1-9,13H

InchiKey: NBTGDHBAHMODDU-UHFFFAOYSA-N

Formula: C14H10BrCl3

SMILES: ClC(Cl)(Cl)C(c1ccccc1)c1ccc(Br)cc1

Mol. weight [g/mol]: 364.49

CAS: 39211-93-3

Physical Properties

Property code	Value	Unit	Source
gf	261.12	kJ/mol	Joback Method
hf	94.38	kJ/mol	Joback Method
hfus	26.65	kJ/mol	Joback Method
hvap	69.88	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	5.951		Crippen Method
mcvol	214.820	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
tb	752.84	K	Joback Method
tc	1034.03	K	Joback Method
tf	449.88	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.28	J/molxK	752.84	Joback Method
cpg	535.24	J/molxK	987.17	Joback Method
cpg	526.99	J/molxK	940.30	Joback Method
cpg	518.07	J/molxK	893.44	Joback Method
cpg	508.28	J/molxK	846.57	Joback Method
cpg	497.41	J/molxK	799.71	Joback Method
cpg	542.99	J/molxK	1034.03	Joback Method
dvisc	0.0000955	Paxs	752.84	Joback Method
dvisc	0.0001238	Paxs	702.35	Joback Method

dvisc	0.0001671	Paxs	651.85	Joback Method
dvisc	0.0002373	Paxs	601.36	Joback Method
dvisc	0.0003593	Paxs	550.87	Joback Method
dvisc	0.0005915	Paxs	500.37	Joback Method
dvisc	0.0010891	Paxs	449.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39211933&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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