

DPE

Other names:	Benzene, 1,1'-(2,2,2-trichloroethylidene)bis- 1,1'-(2,2,2-trichloroethylidene)dibenzene
Inchi:	InChI=1S/C14H11Cl3/c15-14(16,17)13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13H
InchiKey:	ZADGQTHIZZOKGE-UHFFFAOYSA-N
Formula:	C14H11Cl3
SMILES:	<chem>C1C(Cl)(Cl)C(c1ccccc1)c1ccccc1</chem>
Mol. weight [g/mol]:	285.60
CAS:	2971-22-4

Physical Properties

Property code	Value	Unit	Source
gf	256.43	kJ/mol	Joback Method
hf	79.52	kJ/mol	Joback Method
hfus	21.75	kJ/mol	Joback Method
hvap	62.78	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.189		Crippen Method
mcvol	197.320	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tb	681.70	K	Joback Method
tc	951.93	K	Joback Method
tf	377.56	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.16	J/molxK	681.70	Joback Method
cpg	514.27	J/molxK	906.89	Joback Method
cpg	504.79	J/molxK	861.85	Joback Method
cpg	494.32	J/molxK	816.81	Joback Method
cpg	482.66	J/molxK	771.78	Joback Method

cpg	469.67	J/mol×K	726.74	Joback Method
cpg	522.90	J/mol×K	951.93	Joback Method
dvisc	0.0001183	Paxs	681.70	Joback Method
dvisc	0.0001587	Paxs	631.01	Joback Method
dvisc	0.0002239	Paxs	580.32	Joback Method
dvisc	0.0003375	Paxs	529.63	Joback Method
dvisc	0.0005548	Paxs	478.94	Joback Method
dvisc	0.0010260	Paxs	428.25	Joback Method
dvisc	0.0022381	Paxs	377.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2971224&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
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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