Benzene, 1,1'-(2,2,2-trichloroethylidene)bis(4-methyl-

Other names: 2,2-bis-(4-Methylphenyl)-1,1,1-trichloroethane
Inchi: InChI=1S/C16H15Cl3/c1-11-3-7-13(8-4-11)15(16(17,18)19)14-9-5-12(2)6-10-14/h3-10,15
InchiKey: OEMKCHJUXPTUHW-UHFFFAOYSA-N
Formula: C16H15Cl3
SMILES: Cc1ccc(C(c2ccc(C)cc2)C(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]: 313.65
CAS: 4413-31-4

Physical Properties

Property code	Value	Unit	Source
gf	254.01	kJ/mol	Joback Method
hf	15.30	kJ/mol	Joback Method
hfus	26.15	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.806		Crippen Method
mcvol	225.500	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	737.42	K	Joback Method
tc	996.33	K	Joback Method
tf	425.14	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.37	J/mol×K	737.42	Joback Method
cpg	618.07	J/mol×K	953.18	Joback Method
cpg	607.66	J/mol×K	910.03	Joback Method
cpg	596.32	J/mol×K	866.88	Joback Method
cpg	583.91	J/mol×K	823.72	Joback Method
cpg	570.31	J/mol×K	780.57	Joback Method

cpg	627.69	J/mol×K	996.33	Joback Method
dvisc	0.0000898	Pa×s	737.42	Joback Method
dvisc	0.0001171	Pa×s	685.37	Joback Method
dvisc	0.0001594	Pa×s	633.33	Joback Method
dvisc	0.0002294	Pa×s	581.28	Joback Method
dvisc	0.0003545	Pa×s	529.23	Joback Method
dvisc	0.0006025	Pa×s	477.19	Joback Method
dvisc	0.0011661	Pa×s	425.14	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4413314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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