

Benzene, 1,1'-(2,2-dichloroethylidene)bis[4-ethyl-

Other names:	1,1'-(2,2-Dichloroethylidene)bis(4-ethylbenzene) 1,1-Bis(p-Ethylphenyl)-2,2-dichloroethane 1,1-Dichloro-2,2-bis(4-ethylphenyl)ethane 1,1-Dichloro-2,2-bis(p-ethylphenyl)ethane 1,1-bis-(4-Ethylphenyl)-2,2-dichloroethane 2,2-Bis(p-ethylphenyl)-1,1-dichloroethane 2,2-Dichloro-1,1-bis(p-ethylphenyl)ethane Di(p-ethylphenyl)dichloroethane Diethyl-diphenyl dichloroethane ENT-17082 Ethane, 1,1-dichloro-2,2-bis(p-ethylphenyl)- Ethane, 2,2-bis(p-ethylphenyl)-1,1-dichloro- Ethylan NCI-C02868 Perthane Q 137 p,p'-Ethyl-ddd p,p-Ethyl ddd «alpha», «alpha»--Dichloro-2,2-bis(p-ethylphenyl)ethane Â«alphaÂ», Â«alphaÂ»--Dichloro-2,2-bis(p-ethylphenyl)ethane
Inchi:	InChI=1S/C18H20Cl2/c1-3-13-5-9-15(10-6-13)17(18(19)20)16-11-7-14(4-2)8-12-16/h5-1
InchiKey:	QFMDFTQOJHFVNR-UHFFFAOYSA-N
Formula:	C18H20Cl2
SMILES:	CCc1ccc(C(c2ccc(CC)cc2)C(Cl)Cl)cc1
Mol. weight [g/mol]:	307.26
CAS:	72-56-0

Physical Properties

Property code	Value	Unit	Source
gf	277.50	kJ/mol	Joback Method
hf	-6.77	kJ/mol	Joback Method
hfus	31.03	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Joback Method
log10ws	-7.04		Aqueous Solubility Prediction Method
logp	5.747		Crippen Method
mcvol	241.440	ml/mol	McGowan Method

pc	1777.34	kPa	Joback Method
rinpol	2232.00		NIST Webbook
rinpol	2232.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2167.00		NIST Webbook
rinpol	2167.00		NIST Webbook
ripol	3016.00		NIST Webbook
ripol	3016.00		NIST Webbook
tb	748.54	K	Joback Method
tc	985.89	K	Joback Method
tf	333.00 ± 0.20	K	NIST Webbook
tf	332.17 ± 0.20	K	NIST Webbook
vc	0.913	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.60	J/mol×K	748.54	Joback Method
cpg	652.36	J/mol×K	788.10	Joback Method
cpg	667.85	J/mol×K	827.66	Joback Method
cpg	682.14	J/mol×K	867.21	Joback Method
cpg	695.32	J/mol×K	906.77	Joback Method
cpg	707.47	J/mol×K	946.33	Joback Method
cpg	718.67	J/mol×K	985.89	Joback Method
dvisc	0.0014052	Pa×s	400.34	Joback Method
dvisc	0.0006604	Pa×s	458.37	Joback Method
dvisc	0.0003677	Pa×s	516.41	Joback Method
dvisc	0.0002305	Pa×s	574.44	Joback Method
dvisc	0.0001574	Pa×s	632.47	Joback Method
dvisc	0.0001146	Pa×s	690.51	Joback Method
dvisc	0.0000876	Pa×s	748.54	Joback Method
hfust	23.34	kJ/mol	331.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72560&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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