

BENZENE, 1,1'-(2-METHYL-1-PROPENYLIDENE)BIS-

Other names:	Propene, 2-methyl-1,1-diphenyl- 1,1-Dimethyl-2,2-diphenylethene 1,1-Dimethyl-2,2-diphenylethylene 1,1-Diphenyl-2-methylpropene 1,1-Diphenylisobutylene 2-Methyl-1,1-diphenylpropene
Inchi:	InChI=1S/C16H16/c1-13(2)16(14-9-5-3-6-10-14)15-11-7-4-8-12-15/h3-12H,1-2H3
InchiKey:	JHLNLKYQTWQERE-UHFFFAOYSA-N
Formula:	C16H16
SMILES:	CC(C)=C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	208.30

Physical Properties

Property code	Value	Unit	Source
af	0.4437		Cheméo Relay (1.0)
gf	371.78	kJ/mol	Joback Method
hf	221.86	kJ/mol	Cheméo Relay (1.0)
hfus	22.86	kJ/mol	Joback Method
hvap	73.86	kJ/mol	Cheméo Relay (1.0)
ie	8.00	eV	Cheméo Relay (1.0)
log10ws	-4.83		Cheméo Relay (1.0)
logp	4.528		Crippen Method
mcvol	184.480	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
tb	574.39	K	Cheméo Relay (1.0)
tc	819.02	K	Cheméo Relay (1.0)
tf	318.84	K	Cheméo Relay (1.0)
vc	0.668	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.11	J/mol×K	622.76	Joback Method
cpg	469.87	J/mol×K	664.29	Joback Method

cpg	487.12	J/mol×K	705.82	Joback Method
cpg	502.98	J/mol×K	747.36	Joback Method
cpg	517.57	J/mol×K	788.89	Joback Method
cpg	531.03	J/mol×K	830.42	Joback Method
cpg	543.45	J/mol×K	871.95	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C781339&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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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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