

Benzene, 1,1'-methylenebis[4-methyl-

Other names:	Di-p-tolylmethane 4,4'-Dimethyldiphenylmethane Benzene, 1,1'-methylenebis[4-methyl- p-Ditolylmethane 4',4-Dimethyldiphenylmethane Bis-p-tolylmethane Toluene, p,p'-methylenedi- 4,4'-Ditolylmethane
Inchi:	InChI=1S/C15H16/c1-12-3-7-14(8-4-12)11-15-9-5-13(2)6-10-15/h3-10H,11H2,1-2H3
InchiKey:	HZAWPPRBCALFRN-UHFFFAOYSA-N
Formula:	C15H16
SMILES:	Cc1ccc(Cc2ccc(C)cc2)cc1
Mol. weight [g/mol]:	196.29

Physical Properties

Property code	Value	Unit	Source
af	0.5027		Cheméo Relay (1.0)
gf	280.98	kJ/mol	Joback Method
hf	110.88	kJ/mol	Cheméo Relay (1.0)
hfus	21.91	kJ/mol	Joback Method
hvap	77.36	kJ/mol	Cheméo Relay (1.0)
ie	8.29	eV	Cheméo Relay (1.0)
log10ws	-5.26		Cheméo Relay (1.0)
logp	3.894		Crippen Method
mcvol	174.690	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	566.00 ± 5.00	K	NIST Webbook
tc	788.94	K	Cheméo Relay (1.0)
tf	300.30 ± 1.00	K	NIST Webbook
tf	301.00 ± 3.00	K	NIST Webbook
tf	302.00 ± 2.00	K	NIST Webbook
tf	301.70 ± 1.00	K	NIST Webbook
vc	0.668	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.04	J/mol×K	605.92	Joback Method
cpg	438.73	J/mol×K	645.37	Joback Method
cpg	455.19	J/mol×K	684.82	Joback Method
cpg	470.49	J/mol×K	724.27	Joback Method
cpg	484.68	J/mol×K	763.72	Joback Method
cpg	497.83	J/mol×K	803.17	Joback Method
cpg	510.01	J/mol×K	842.62	Joback Method
dvisc	0.0014790	Pa×s	336.69	Joback Method
dvisc	0.0008204	Pa×s	381.56	Joback Method
dvisc	0.0005152	Pa×s	426.43	Joback Method
dvisc	0.0003535	Pa×s	471.31	Joback Method
dvisc	0.0002590	Pa×s	516.18	Joback Method
dvisc	0.0001994	Pa×s	561.05	Joback Method
dvisc	0.0001596	Pa×s	605.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	438.20	K	1.60	NIST Webbook
tbrp	429.50 ± 1.50	K	2.10	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4957146&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

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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