«alpha»-Methylstilbene

Other names:	1,2-Diphenyl-1-propene
	1,2-Diphenylpropene
	1-Methyl-1,2-diphenylethene
	1-Propene, 1,2-diphenyl-
	Benzene, 1,1'-(1-methyl-1,2-ethenediyl)bis-
	Stilbene, «alpha»-methyl-
	Stilbene, Â«alphaÂ»-methyl-
Inchi:	InChI=1S/C15H14/c1-13(15-10-6-3-7-11-15)12-14-8-4-2-5-9-14/h2-12H,1H3
InchiKey:	OVZXISBUYCEVEV-UHFFFAOYSA-N
Formula:	C15H14
SMILES:	CC(=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	194.27
CAS:	779-51-1

Physical Properties

Property code	Value	Unit	Source
gf	371.91	kJ/mol	Joback Method
hf	227.56	kJ/mol	Joback Method
hfus	21.58	kJ/mol	Joback Method
hvap	53.57	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.247		Crippen Method
mcvol	170.390	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
ripol	2446.00		NIST Webbook
ripol	2446.00		NIST Webbook
tb	558.00 ± 5.00	K	NIST Webbook
tc	850.12	K	Joback Method
tf	355.00 ± 3.00	K	NIST Webbook
tf	354.00 ± 2.00	K	NIST Webbook
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.25	J/mol×K	600.00	Joback Method
cpg	419.27	J/mol×K	641.69	Joback Method
cpg	435.81	J/mol×K	683.37	Joback Method
cpg	450.99	J/mol×K	725.06	Joback Method
cpg	464.92	J/mol×K	766.75	Joback Method
cpg	477.72	J/mol×K	808.43	Joback Method
cpg	489.51	J/mol×K	850.12	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42576e+01
Coeff. B	-4.44896e+03
Coeff. C	-9.64550e+01
Temperature range (K), min.	414.92
Temperature range (K), max.	593.76

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C779511&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume