Benzene, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-, (R*,R*)-(.+/-.)-

Other names: Benzene, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-, (R*,R*)-(±)-
Benzene, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-, (R*,R*)-(Â±)-
Bibenzyl, «alpha»,«alpha»'-dimethyl-, (.+/-.)-
Bibenzyl, «alpha»,«alpha»'-dimethyl-, (±)-
Bibenzyl, «alpha»,«alpha»'-dimethyl-, DL-
Bibenzyl, Â«alphaÂ»,Â«alphaÂ»'-dimethyl-, (.+/-.)-
Bibenzyl, Â«alphaÂ»,Â«alphaÂ»'-dimethyl-, (Â±)-
Bibenzyl, Â«alphaÂ»,Â«alphaÂ»'-dimethyl-, DL-
DL-2,3-Diphenylbutane

Inchi: InChI=1S/C16H18/c1-13(15-9-5-3-6-10-15)14(2)16-11-7-4-8-12-16/h3-14H,1-2H3/t13-,14

InchiKey: NGCFVIRRWORSML-ZIAGYGMSSA-N

Formula: C16H18

SMILES: CC(c1ccccc1)C(C)c1ccccc1

Mol. weight [g/mol]: 210.31

CAS: 2726-21-8

Physical Properties

Property code	Value	Unit	Source
chs	-8933.00	kJ/mol	NIST Webbook
gf	303.78	kJ/mol	Joback Method
hf	88.93	kJ/mol	Joback Method
hfus	18.23	kJ/mol	Joback Method
hvap	54.99	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.594		Crippen Method
mcvol	188.780	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	577.20 ± 0.60	K	NIST Webbook
tc	858.10	K	Joback Method
tf	292.92	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.14	J/mol×K	617.96	Joback Method
cpg	492.74	J/mol×K	657.98	Joback Method
cpg	510.86	J/mol×K	698.01	Joback Method
cpg	527.59	J/mol×K	738.03	Joback Method
cpg	543.01	J/mol×K	778.05	Joback Method
cpg	557.20	J/mol×K	818.08	Joback Method
cpg	570.27	J/mol×K	858.10	Joback Method
dvisc	0.0044099	Pa×s	292.92	Joback Method
dvisc	0.0015524	Pa×s	347.09	Joback Method
dvisc	0.0007244	Pa×s	401.27	Joback Method
dvisc	0.0004053	Pa×s	455.44	Joback Method
dvisc	0.0002565	Pa×s	509.61	Joback Method
dvisc	0.0001773	Pa×s	563.79	Joback Method
dvisc	0.0001307	Pa×s	617.96	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42898e+01
Coeff. B	-4.60742e+03
Coeff. C	-1.01612e+02
Temperature range (K), min.	430.66
Temperature range (K), max.	614.78

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2726218&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

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

Legend

chs:	Standard solid enthalpy of combustion
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume