

Benzene, 1,1'-(1,5-hexadiene-1,6-diyl)bis-

Other names:	1,6-diphenyl-1,5-hexadiene
Inchi:	InChI=1S/C18H18/c1(5-11-17-13-7-3-8-14-17)2-6-12-18-15-9-4-10-16-18/h3-16H,1-2H2
InchiKey:	GXBNHFMSIXKWHZ-YDWXAUTNSA-N
Formula:	C18H18
SMILES:	<chem>C(=Cc1ccccc1)CCC=Cc1ccccc1</chem>
Mol. weight [g/mol]:	234.34
CAS:	4439-45-6

Physical Properties

Property code	Value	Unit	Source
gf	485.94	kJ/mol	Joback Method
hf	292.65	kJ/mol	Joback Method
hfus	30.86	kJ/mol	Joback Method
hvap	60.13	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.193		Crippen Method
mcvol	208.360	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
tb	672.92	K	Joback Method
tc	913.05	K	Joback Method
tf	335.30	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.84	J/molxK	672.92	Joback Method
cpg	552.08	J/molxK	712.94	Joback Method
cpg	568.92	J/molxK	752.96	Joback Method
cpg	584.48	J/molxK	792.99	Joback Method
cpg	598.90	J/molxK	833.01	Joback Method
cpg	612.31	J/molxK	873.03	Joback Method
cpg	624.86	J/molxK	913.05	Joback Method
dvisc	0.0018943	Paxs	335.30	Joback Method

dvisc	0.0007954	Paxs	391.57	Joback Method
dvisc	0.0004154	Paxs	447.84	Joback Method
dvisc	0.0002508	Paxs	504.11	Joback Method
dvisc	0.0001675	Paxs	560.38	Joback Method
dvisc	0.0001205	Paxs	616.65	Joback Method
dvisc	0.0000916	Paxs	672.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4439456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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