Benzene, 1,1'-(1,3,5,7-octatetraene-1,8-diyl)bis-, (all-E)-

Other names: 1,3,5,7-Octatetraene, 1,8-diphenyl-, (all-E)-
All-trans-Diphenyloctatetraene
Benzene,1,1'-(1,3,5,7-octatetraene-1,8-diyl)bis-

Inchi: InChI=1S/C20H18/c1(3-7-13-19-15-9-5-10-16-19)2-4-8-14-20-17-11-6-12-18-20/h1-18H/

InchiKey: ZENGMMQJMCPHTK-FPPPDJHPSA-N

Formula: C20H18

SMILES: C(C=CC=Cc1ccccc1)=CC=Cc1ccccc1

Mol. weight [g/mol]: 258.36

CAS: 22828-29-1

Physical Properties

Property code	Value	Unit	Source
gf	663.22	kJ/mol	Joback Method
hf	485.81	kJ/mol	Joback Method
hfus	36.45	kJ/mol	Joback Method
hvap	64.50	kJ/mol	Joback Method
ie	7.19	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-6.15		Crippen Method
logp	5.526		Crippen Method
mcvol	227.940	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
tb	727.00	K	Joback Method
tc	976.35	K	Joback Method
tf	347.68	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.66	J/mol×K	727.00	Joback Method
cpg	612.29	J/mol×K	768.56	Joback Method
cpg	628.58	J/mol×K	810.12	Joback Method
cpg	643.75	J/mol×K	851.68	Joback Method

cpg	658.00	J/mol×K	893.24	Joback Method
cpg	671.53	J/mol×K	934.80	Joback Method
cpg	684.53	J/mol×K	976.35	Joback Method
dvisc	0.0014282	Pa×s	347.68	Joback Method
dvisc	0.0005478	Pa×s	410.90	Joback Method
dvisc	0.0002713	Pa×s	474.12	Joback Method
dvisc	0.0001585	Pa×s	537.34	Joback Method
dvisc	0.0001037	Pa×s	600.56	Joback Method
dvisc	0.0000736	Pa×s	663.78	Joback Method
dvisc	0.0000554	Pa×s	727.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22828291&Units=SI
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

Legend

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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