Benzene, 1,3-hexadienyl-

Other names: Hexa-1,3-dienylbenzene
1,3-hexadienylbenzene
Inchi: InChI=1S/C12H14/c1-2-3-4-6-9-12-10-7-5-8-11-12/h3-11H,2H2,1H3/b4-3+,9-6+
InchiKey: DHGJWSRGFMFRLS-JAFPNSLJSA-N
Formula: C12H14
SMILES: CCC=CC=Cc1ccccc1
Mol. weight [g/mol]: 158.24
CAS: 41635-77-2

Physical Properties

Property code	Value	Unit	Source
gf	323.01	kJ/mol	Joback Method
hf	179.96	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	44.50	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.666		Crippen Method
mcvol	147.580	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
tb	508.96	K	Joback Method
tc	727.68	K	Joback Method
tf	241.26	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.85	J/mol×K	508.96	Joback Method
cpg	326.97	J/mol×K	545.41	Joback Method
cpg	341.98	J/mol×K	581.87	Joback Method
cpg	355.97	J/mol×K	618.32	Joback Method
cpg	368.99	J/mol×K	654.77	Joback Method
cpg	381.14	J/mol×K	691.22	Joback Method
cpg	392.47	J/mol×K	727.68	Joback Method

dvisc	0.0033122	Pa×s	241.26	Joback Method
dvisc	0.0013165	Pa×s	285.88	Joback Method
dvisc	0.0006713	Pa×s	330.49	Joback Method
dvisc	0.0004018	Pa×s	375.11	Joback Method
dvisc	0.0002682	Pa×s	419.73	Joback Method
dvisc	0.0001935	Pa×s	464.34	Joback Method
dvisc	0.0001478	Pa×s	508.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41635772&Units=SI

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
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