HEXA-2,4-DIENYLBENZENE

Other names: 2,4-Hexadienylbenzene
6-Phenyl-2,4-hexadiene
Inchi: InChI=1S/C12H14/c1-2-3-4-6-9-12-10-7-5-8-11-12/h2-8,10-11H,9H2,1H3/b3-2-,6-4+
InchiKey: JSQZPUUCMYDLKO-ZPYFUIHZSA-N
Formula: C12H14
SMILES: C/C=C/C=C\Cc1ccccc1
Mol. weight [g/mol]: 158.24

Physical Properties

Property code	Value	Unit	Source
hfus	21.28	kJ/mol	Joback Method
hvap	60.45	kJ/mol	Cheméo Relay (1.0)
ie	8.29	eV	Cheméo Relay (1.0)
logp	3.361		Crippen Method
mcvol	147.580	ml/mol	McGowan Method
rinpol	1517.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1446.00		NIST Webbook
tb	497.45	K	Cheméo Relay (1.0)
tf	236.57	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79482863&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point