

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:	CC=CC=CCc1ccccc1
Mol. weight [g/mol]:	158.24
CAS:	79482-86-3

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	-3.66		Crippen Method
logp	3.361		Crippen Method
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

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

Sources

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=C79482863&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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