2,6-Diphenyl-1,6-heptadiene

Other names: 1,6-Heptadiene, 2,6-diphenyl-
(1-Methylene-5-phenyl-5-hexenyl)benzene
Inchi: InChI=1S/C19H20/c1-16(18-12-5-3-6-13-18)10-9-11-17(2)19-14-7-4-8-15-19/h3-8,12-15H
InchiKey: IADWADXXRTZWQV-UHFFFAOYSA-N
Formula: C19H20
SMILES: C=C(CCCC(=C)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 248.36
CAS: 27905-65-3

Physical Properties

Property code	Value	Unit	Source
gf	492.50	kJ/mol	Joback Method
hf	259.00	kJ/mol	NIST Webbook
hfus	27.87	kJ/mol	Joback Method
hvap	61.26	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.583		Crippen Method
mcvol	222.450	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
tb	680.60	K	Joback Method
tc	914.37	K	Joback Method
tf	325.29	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.68	J/mol×K	680.60	Joback Method
cpg	603.64	J/mol×K	719.56	Joback Method
cpg	621.18	J/mol×K	758.52	Joback Method
cpg	637.41	J/mol×K	797.49	Joback Method
cpg	652.45	J/mol×K	836.45	Joback Method
cpg	666.40	J/mol×K	875.41	Joback Method
cpg	679.37	J/mol×K	914.37	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=C27905653&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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