

Hexane, 3,4-diphenyl-

Inchi:	InChI=1S/C18H22/c1-3-17(15-11-7-5-8-12-15)18(4-2)16-13-9-6-10-14-16/h5-14,17-18H,
InchiKey:	JTJWVUQPSOFEPZ-UHFFFAOYSA-N
Formula:	C18H22
SMILES:	CCC(c1ccccc1)C(CC)c1ccccc1
Mol. weight [g/mol]:	238.37
CAS:	5789-31-1

Physical Properties

Property code	Value	Unit	Source
gf	320.62	kJ/mol	Joback Method
hf	47.65	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	59.44	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.374		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
tb	571.00 ± 5.00	K	NIST Webbook
tc	894.23	K	Joback Method
tf	365.00 ± 4.00	K	NIST Webbook
vc	0.816	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.75	J/mol×K	663.72	Joback Method
cpg	598.84	J/mol×K	702.14	Joback Method
cpg	617.48	J/mol×K	740.56	Joback Method
cpg	634.76	J/mol×K	778.98	Joback Method
cpg	650.76	J/mol×K	817.40	Joback Method
cpg	665.57	J/mol×K	855.81	Joback Method
cpg	679.28	J/mol×K	894.23	Joback Method
dvisc	0.0037813	Paxs	315.46	Joback Method
dvisc	0.0013126	Paxs	373.50	Joback Method

dvisc	0.0006057	Paxs	431.55	Joback Method
dvisc	0.0003357	Paxs	489.59	Joback Method
dvisc	0.0002109	Paxs	547.63	Joback Method
dvisc	0.0001448	Paxs	605.68	Joback Method
dvisc	0.0001062	Paxs	663.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C5789311&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

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