

2,3-diphenyl-3-hexene

Inchi:	InChI=1S/C18H20/c1-3-10-18(17-13-8-5-9-14-17)15(2)16-11-6-4-7-12-16/h4-15H,3H2,1-
InchiKey:	MSVPALSZRZMLFS-ZDLGFXPLSA-N
Formula:	C18H20
SMILES:	CCC=C(c1ccccc1)C(C)c1ccccc1
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	394.73	kJ/mol	Joback Method
hf	160.36	kJ/mol	Joback Method
hfus	25.83	kJ/mol	Joback Method
hvap	59.86	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.284		Crippen Method
mcvol	212.660	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1880.00		NIST Webbook
tb	668.20	K	Joback Method
tc	907.56	K	Joback Method
tf	311.42	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.15	J/mol×K	668.20	Joback Method
cpg	575.62	J/mol×K	708.09	Joback Method
cpg	593.63	J/mol×K	747.99	Joback Method
cpg	610.27	J/mol×K	787.88	Joback Method
cpg	625.66	J/mol×K	827.77	Joback Method
cpg	639.92	J/mol×K	867.66	Joback Method
cpg	653.17	J/mol×K	907.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316297&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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