

2,4-Diphenyl-4-methyl-2(E)-pentene

Other names:	(E)-(4-Methylpent-2-ene-2,4-diyl)dibenzene
Inchi:	InChI=1S/C18H20/c1-15(16-10-6-4-7-11-16)14-18(2,3)17-12-8-5-9-13-17/h4-14H,1-3H3/
InchiKey:	VOOVDZMAQQVAEW-CCEZHUSRSA-N
Formula:	C18H20
SMILES:	CC(=CC(C)(C)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	236.35
CAS:	22768-22-5

Physical Properties

Property code	Value	Unit	Source
gf	400.01	kJ/mol	Joback Method
hf	156.89	kJ/mol	Joback Method
hfus	21.94	kJ/mol	Joback Method
hvap	58.96	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	5.068		Crippen Method
mcvol	212.660	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1836.10		NIST Webbook
rinpol	1836.10		NIST Webbook
tb	665.41	K	Joback Method
tc	914.25	K	Joback Method
tf	328.84	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.41	J/molxK	665.41	Joback Method
cpg	578.36	J/molxK	706.88	Joback Method
cpg	596.66	J/molxK	748.36	Joback Method
cpg	613.47	J/molxK	789.83	Joback Method
cpg	628.95	J/molxK	831.30	Joback Method
cpg	643.25	J/molxK	872.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22768225&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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