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: C/C(=C\C(C)(C)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 236.36

Physical Properties

Property code	Value	Unit	Source
af	0.4222		Cheméo Relay (1.0)
hf	203.33	kJ/mol	Cheméo Relay (1.0)
hfus	21.94	kJ/mol	Joback Method
hvap	85.90	kJ/mol	Cheméo Relay (1.0)
ie	7.92	eV	Cheméo Relay (1.0)
log10ws	-5.94		Cheméo Relay (1.0)
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	587.20	K	Cheméo Relay (1.0)
tc	826.53	K	Cheméo Relay (1.0)
tf	313.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.41	J/mol×K	665.41	Joback Method
cpg	578.36	J/mol×K	706.88	Joback Method
cpg	596.66	J/mol×K	748.36	Joback Method
cpg	613.47	J/mol×K	789.83	Joback Method
cpg	628.95	J/mol×K	831.30	Joback Method
cpg	643.25	J/mol×K	872.77	Joback Method
cpg	656.55	J/mol×K	914.25	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22768225&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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