

2,4-diphenyl-1-butene

Other names:	1-Butene, 2,4-diphenyl
Inchi:	InChI=1S/C16H16/c1-14(16-10-6-3-7-11-16)12-13-15-8-4-2-5-9-15/h2-11H,1,12-13H2
InchiKey:	PWSZACWUDDFZMQ-UHFFFAOYSA-N
Formula:	C16H16
SMILES:	<chem>C=C(Cc1ccccc1)c1ccccc1</chem>
Mol. weight [g/mol]:	208.30

Physical Properties

Property code	Value	Unit	Source
gf	387.95	kJ/mol	Joback Method
hf	215.13	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	55.17	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.333		Crippen Method
mcvol	184.480	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1710.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1691.00		NIST Webbook
tb	615.40	K	Joback Method
tc	854.69	K	Joback Method
tf	307.20	K	Joback Method
vc	0.698	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	450.45	J/mol×K	615.40	Joback Method
cpg	468.83	J/mol×K	655.28	Joback Method
cpg	485.80	J/mol×K	695.16	Joback Method
cpg	501.46	J/mol×K	735.05	Joback Method
cpg	515.89	J/mol×K	774.93	Joback Method
cpg	529.19	J/mol×K	814.81	Joback Method
cpg	541.46	J/mol×K	854.69	Joback Method

Sources

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=R72749&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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