

1,4-diphenyl-1-butene

Inchi:	InChI=1S/C17H18/c1-15(17-13-6-3-7-14-17)9-8-12-16-10-4-2-5-11-16/h2-8,10-15H,9H2,
InchiKey:	KKSPSCQACIDIMM-XYOKQWHBSA-N
Formula:	C17H18
SMILES:	CC(CC=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	222.32

Physical Properties

Property code	Value	Unit	Source
gf	394.86	kJ/mol	Joback Method
hf	190.79	kJ/mol	Joback Method
hfus	24.55	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.894		Crippen Method
mcvol	198.570	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1731.10		NIST Webbook
rinpol	1734.10		NIST Webbook
rinpol	1731.10		NIST Webbook
tb	645.44	K	Joback Method
tc	885.65	K	Joback Method
tf	314.11	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.60	J/molxK	645.44	Joback Method
cpg	584.77	J/molxK	845.62	Joback Method
cpg	571.01	J/molxK	805.58	Joback Method
cpg	556.13	J/molxK	765.55	Joback Method
cpg	540.01	J/molxK	725.51	Joback Method
cpg	522.53	J/molxK	685.48	Joback Method
cpg	597.51	J/molxK	885.65	Joback Method

dvisc	0.0001092	Paxs	645.44	Joback Method
dvisc	0.0001457	Paxs	590.22	Joback Method
dvisc	0.0002065	Paxs	535.00	Joback Method
dvisc	0.0003170	Paxs	479.78	Joback Method
dvisc	0.0005439	Paxs	424.55	Joback Method
dvisc	0.0010970	Paxs	369.33	Joback Method
dvisc	0.0028316	Paxs	314.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316059&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

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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