

1-Butene, 1,4-diphenyl #1

Inchi:	InChI=1S/C16H16/c1-3-9-15(10-4-1)13-7-8-14-16-11-5-2-6-12-16/h1-7,9-13H,8,14H2/b1
InchiKey:	NJJOGKAWAWZLAU-QPEQYQDCSA-N
Formula:	C16H16
SMILES:	C(=Cc1ccccc1)CCc1ccccc1
Mol. weight [g/mol]:	208.30

Physical Properties

Property code	Value	Unit	Source
gf	388.88	kJ/mol	Joback Method
hf	216.71	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.333		Crippen Method
mcvol	184.480	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
tb	623.00	K	Joback Method
tc	863.17	K	Joback Method
tf	317.84	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.62	J/molxK	623.00	Joback Method
cpg	469.78	J/molxK	663.03	Joback Method
cpg	486.53	J/molxK	703.06	Joback Method
cpg	501.97	J/molxK	743.09	Joback Method
cpg	516.22	J/molxK	783.11	Joback Method
cpg	529.37	J/molxK	823.14	Joback Method
cpg	541.54	J/molxK	863.17	Joback Method
dvisc	0.0022682	Paxs	317.84	Joback Method

dvisc	0.0010118	Paxs	368.70	Joback Method
dvisc	0.0005489	Paxs	419.56	Joback Method
dvisc	0.0003399	Paxs	470.42	Joback Method
dvisc	0.0002311	Paxs	521.28	Joback Method
dvisc	0.0001683	Paxs	572.14	Joback Method
dvisc	0.0001290	Paxs	623.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R72927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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