

Benzene, (1,1-dimethyl-2-propenyl)-

Other names:	1-Butene, 3-methyl-3-phenyl- 3-Methyl-3-phenyl-1-butene
Inchi:	InChI=1S/C11H14/c1-4-11(2,3)10-8-6-5-7-9-10/h4-9H,1H2,2-3H3
InchiKey:	DKOQCZJPMFXMKH-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	C=CC(C)(C)c1ccccc1
Mol. weight [g/mol]:	146.23
CAS:	18321-36-3

Physical Properties

Property code	Value	Unit	Source
gf	244.83	kJ/mol	Joback Method
hf	82.84	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	40.39	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.150		Crippen Method
mvol	137.790	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	471.21	K	Joback Method
tc	691.62	K	Joback Method
tf	240.81	K	Joback Method
vc	0.513	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.21	J/molxK	471.21	Joback Method
cpg	358.56	J/molxK	654.89	Joback Method
cpg	346.00	J/molxK	618.15	Joback Method
cpg	332.46	J/molxK	581.42	Joback Method
cpg	317.86	J/molxK	544.68	Joback Method
cpg	302.13	J/molxK	507.95	Joback Method
cpg	370.19	J/molxK	691.62	Joback Method

dvisc	0.0002189	Paxs	471.21	Joback Method
dvisc	0.0002934	Paxs	432.81	Joback Method
dvisc	0.0004163	Paxs	394.41	Joback Method
dvisc	0.0006369	Paxs	356.01	Joback Method
dvisc	0.0010799	Paxs	317.61	Joback Method
dvisc	0.0021175	Paxs	279.21	Joback Method
dvisc	0.0051466	Paxs	240.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18321363&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
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:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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