BENZENE, (1-METHYL-2-PROPENYL)-

Other names: 1-Methyl-2-propenyl)-benzene
3-phenyl-1-butene
Inchi: InChI=1S/C10H12/c1-3-9(2)10-7-5-4-6-8-10/h3-9H,1H2,2H3
InchiKey: CHPXLAPHLQIKCA-UHFFFAOYSA-N
Formula: C10H12
SMILES: C=CC(C)c1ccccc1
Mol. weight [g/mol]: 132.21

Physical Properties

Property code	Value	Unit	Source
af	0.2660		Cheméo Relay (1.0)
gf	231.13	kJ/mol	Joback Method
hf	107.08	kJ/mol	Cheméo Relay (1.0)
hfus	10.89	kJ/mol	Joback Method
hvap	47.97	kJ/mol	Cheméo Relay (1.0)
ie	8.59	eV	Cheméo Relay (1.0)
log10ws	-3.25		Cheméo Relay (1.0)
logp	2.976		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1114.80		NIST Webbook
tb	439.65	K	Cheméo Relay (1.0)
tc	644.72	K	Cheméo Relay (1.0)
tf	203.39	K	Cheméo Relay (1.0)
vc	0.445	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.82	J/mol×K	451.12	Joback Method
cpg	254.75	J/mol×K	486.82	Joback Method
cpg	268.77	J/mol×K	522.52	Joback Method
cpg	281.92	J/mol×K	558.22	Joback Method
cpg	294.24	J/mol×K	593.92	Joback Method

cpg	305.77	J/mol×K	629.62	Joback Method
cpg	316.54	J/mol×K	665.32	Joback Method
dvisc	0.0050043	Pa×s	212.12	Joback Method
dvisc	0.0019593	Pa×s	251.95	Joback Method
dvisc	0.0009909	Pa×s	291.79	Joback Method
dvisc	0.0005904	Pa×s	331.62	Joback Method
dvisc	0.0003930	Pa×s	371.45	Joback Method
dvisc	0.0002831	Pa×s	411.29	Joback Method
dvisc	0.0002161	Pa×s	451.12	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C934101&Units=SI

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):

Legend

af: Acentric Factor
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
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

vc: Critical Volume