

Benzene, (1-methyl-1-butenyl)-, E

Inchi:	InChI=1S/C11H14/c1-3-7-10(2)11-8-5-4-6-9-11/h4-9H,3H2,1-2H3/b10-7+
InchiKey:	PLPHXVSTHYOUJO-JXMROGBWSA-N
Formula:	C11H14
SMILES:	CCC=C(C)c1ccccc1
Mol. weight [g/mol]:	146.23
CAS:	70303-28-5

Physical Properties

Property code	Value	Unit	Source
gf	225.82	kJ/mol	Joback Method
hf	73.59	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	42.39	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.500		Crippen Method
mcvol	137.790	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1184.00		NIST Webbook
tb	481.80	K	Joback Method
tc	697.83	K	Joback Method
tf	221.11	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.15	J/mol×K	481.80	Joback Method
cpg	299.13	J/mol×K	517.81	Joback Method
cpg	314.10	J/mol×K	553.81	Joback Method
cpg	328.12	J/mol×K	589.82	Joback Method
cpg	341.24	J/mol×K	625.82	Joback Method
cpg	353.51	J/mol×K	661.83	Joback Method
cpg	364.98	J/mol×K	697.83	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=C70303285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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