Benzene, (1-methylenepropyl)-

Other names:	(1-METHYLENEPROPYL)BENZENE
	1-Butene, 2-phenyl-
	2-Phenyl-1-butene
	ALPHA-ETHYLSTYRENE
	Styrene, «alpha»-ethyl-
	Styrene, Â«alphaÂ»-ethyl-
	«alpha»-Ethylstyrene
	Â«alphaÂ»-Ethylstyrene
Inchi:	InChI=1S/C10H12/c1-3-9(2)10-7-5-4-6-8-10/h4-8H,2-3H2,1H3
InchiKey:	SQHOHKQMTHROSF-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	C=C(CC)c1ccccc1
Mol. weight [g/mol]:	132.20
CAS:	2039-93-2

Physical Properties

Property code	Value	Unit	Source
gf	225.02	kJ/mol	Joback Method
hf	102.44	kJ/mol	Joback Method
hfus	13.11	kJ/mol	Joback Method
hvap	51.80 ± 0.30	kJ/mol	NIST Webbook
log10ws	-3.13		Crippen Method
logp	3.110		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	1058.40		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1058.40		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1058.40		NIST Webbook
tb	455.15 ± 2.00	K	NIST Webbook
tb	452.65 ± 2.00	K	NIST Webbook
tb	454.15 ± 2.00	K	NIST Webbook
tb	455.20	K	NIST Webbook
tb	453.00 ± 3.00	K	NIST Webbook

tc	664.84	K	Joback Method
tf	213.16	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.63	J/mol×K	451.44	Joback Method
cpg	254.37	J/mol×K	487.01	Joback Method
cpg	268.22	J/mol×K	522.57	Joback Method
cpg	281.21	J/mol×K	558.14	Joback Method
cpg	293.39	J/mol×K	593.71	Joback Method
cpg	304.80	J/mol×K	629.28	Joback Method
cpg	315.48	J/mol×K	664.84	Joback Method
hvapt	52.00 ± 0.30	kJ/mol	293.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2039932&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
KDB: https://www.cheric.org/files/research/kdb/mol/mol727.mol

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
hvapt: Enthalpy of vaporization at a given temperature
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