Benzene, 1,3-butadienyl-

Other names:	1,3-Butadiene, 1-phenyl-
	1-Phenylbutadiene
	1-Phenyl-1,3-butadiene
	1,3-Butadienylbenzene
Inchi:	InChI=1S/C10H10/c1-2-3-7-10-8-5-4-6-9-10/h2-9H,1H2
InchiKey:	XZKRXPZXQLARHH-UHFFFAOYSA-N
Formula:	C10H10
SMILES:	C=CC=Cc1ccccc1
Mol. weight [g/mol]:	130.19
CAS:	1515-78-2

Physical Properties

Property code	Value	Unit	Source
gf	313.79	kJ/mol	Joback Method
hf	229.45	kJ/mol	Joback Method
hfus	14.62	kJ/mol	Joback Method
hvap	39.42	kJ/mol	Joback Method
ie	8.39	eV	NIST Webbook
log10ws	-2.99		Crippen Method
logp	2.886		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	177.00		NIST Webbook
rinpol	1150.00		NIST Webbook
ripol	1572.00		NIST Webbook
tb	455.72	K	Joback Method
tc	675.61	K	Joback Method
tf	222.04	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.50	J/mol×K	455.72	Joback Method

cpg	237.60	J/mol×K	492.37	Joback Method
cpg	250.71	J/mol×K	529.02	Joback Method
cpg	262.90	J/mol×K	565.67	Joback Method
cpg	274.22	J/mol×K	602.32	Joback Method
cpg	284.74	J/mol×K	638.97	Joback Method
cpg	294.51	J/mol×K	675.61	Joback Method
dvisc	0.0030060	Pa×s	222.04	Joback Method
dvisc	0.0013450	Pa×s	260.99	Joback Method
dvisc	0.0007416	Pa×s	299.93	Joback Method
dvisc	0.0004689	Pa×s	338.88	Joback Method
dvisc	0.0003258	Pa×s	377.83	Joback Method
dvisc	0.0002424	Pa×s	416.77	Joback Method
dvisc	0.0001896	Pa×s	455.72	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C1515782&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume