

Benzene, (2-iodoethenyl)-

Other names:	(2-iodoethenyl)benzene
Inchi:	InChI=1S/C8H7I/c9-7-6-8-4-2-1-3-5-8/h1-7H/b7-6+
InchiKey:	OZPOYKXYJOHGCV-VOTSOKGWSA-N
Formula:	C8H7I
SMILES:	IC=Cc1cccc1
Mol. weight [g/mol]:	230.05
CAS:	101349-79-5

Physical Properties

Property code	Value	Unit	Source
gf	267.23	kJ/mol	Joback Method
hf	222.17	kJ/mol	Joback Method
hfus	15.13	kJ/mol	Joback Method
hvap	45.01	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.092		Crippen Method
mcvol	121.340	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	506.42	K	Joback Method
tc	766.03	K	Joback Method
tf	259.32	K	Joback Method
vc	0.444	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.63	J/molxK	506.42	Joback Method
cpg	217.17	J/molxK	549.69	Joback Method
cpg	227.65	J/molxK	592.96	Joback Method
cpg	237.16	J/molxK	636.22	Joback Method
cpg	245.81	J/molxK	679.49	Joback Method
cpg	253.68	J/molxK	722.76	Joback Method
cpg	260.87	J/molxK	766.03	Joback Method
dvisc	0.0038491	Paxs	259.32	Joback Method

dvisc	0.0018089	Paxs	300.50	Joback Method
dvisc	0.0010198	Paxs	341.69	Joback Method
dvisc	0.0006504	Paxs	382.87	Joback Method
dvisc	0.0004527	Paxs	424.05	Joback Method
dvisc	0.0003359	Paxs	465.24	Joback Method
dvisc	0.0002617	Paxs	506.42	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=C101349795&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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