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: OZPOYKXYJOHGCW-VOTSOKGWSA-N
Formula: C8H7I
SMILES: I/C=C/c1ccccc1
Mol. weight [g/mol]: 230.05

Physical Properties

Property code	Value	Unit	Source
af	0.2648		Cheméo Relay (1.0)
gf	267.23	kJ/mol	Joback Method
hf	235.27	kJ/mol	Cheméo Relay (1.0)
hfus	15.13	kJ/mol	Joback Method
hvap	59.96	kJ/mol	Cheméo Relay (1.0)
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-3.89		Cheméo Relay (1.0)
logp	3.092		Crippen Method
mcvol	121.340	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	527.67	K	Cheméo Relay (1.0)
tc	770.56	K	Cheméo Relay (1.0)
tf	292.60	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0018089	Pa×s	300.50	Joback Method
dvisc	0.0010198	Pa×s	341.69	Joback Method
dvisc	0.0006504	Pa×s	382.87	Joback Method
dvisc	0.0004527	Pa×s	424.05	Joback Method
dvisc	0.0003359	Pa×s	465.24	Joback Method
dvisc	0.0002617	Pa×s	506.42	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C101349795&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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

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