

Benzene, 2-ethenyl-1,3,5-trimethyl-

Other names:	Styrene, 2,4,6-trimethyl- Mesitylethylene Vinylmesitylene 2-Vinylmesitylene 2,4,6-Trimethylstyrene 1,3,5-Trimethyl-2-vinylbenzene
Inchi:	InChI=1S/C11H14/c1-5-11-9(3)6-8(2)7-10(11)4/h5-7H,1H2,2-4H3
InchiKey:	PDELBHCVXBSVPJ-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	<chem>C=Cc1c(C)cc(C)cc1C</chem>
Mol. weight [g/mol]:	146.23
CAS:	769-25-5

Physical Properties

Property code	Value	Unit	Source
gf	213.10	kJ/mol	Joback Method
hf	57.18	kJ/mol	Joback Method
hfus	15.84	kJ/mol	Joback Method
hvap	43.67	kJ/mol	Joback Method
ie	8.33	eV	NIST Webbook
log10ws	-3.72		Crippen Method
logp	3.255		Crippen Method
mcvol	137.790	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
tb	482.20	K	NIST Webbook
tb	477.00 ± 5.00	K	NIST Webbook
tc	699.55	K	Joback Method
tf	236.15 ± 0.50	K	NIST Webbook
vc	0.524	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.33	J/mol×K	489.38	Joback Method

cpg	298.54	J/mol×K	524.41	Joback Method
cpg	312.04	J/mol×K	559.44	Joback Method
cpg	324.86	J/mol×K	594.46	Joback Method
cpg	337.01	J/mol×K	629.49	Joback Method
cpg	348.52	J/mol×K	664.52	Joback Method
cpg	359.41	J/mol×K	699.55	Joback Method
dvisc	0.0012252	Paxs	275.95	Joback Method
dvisc	0.0007579	Paxs	311.52	Joback Method
dvisc	0.0005173	Paxs	347.09	Joback Method
dvisc	0.0003791	Paxs	382.67	Joback Method
dvisc	0.0002929	Paxs	418.24	Joback Method
dvisc	0.0002357	Paxs	453.81	Joback Method
dvisc	0.0001957	Paxs	489.38	Joback Method
hvapt	50.90	kJ/mol	422.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C769255&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvapt:	Enthalpy of vaporization at a given temperature
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
vc: Critical Volume

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