

Benzene, 1-(1,1-dimethylethyl)-4-ethenyl-

Other names:	1-(1,1-Dimethylethyl)-4-ethenylbenzene 4-tert-Butylstyrene Styrene, p-tert-butyl- p-t-Butylstyrene p-tert-Butylstyrene
Inchi:	InChI=1S/C12H16/c1-5-10-6-8-11(9-7-10)12(2,3)4/h5-9H,1H2,2-4H3
InchiKey:	QEDJMOONZLUIMC-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	<chem>C=Cc1ccc(C(C)(C)C)cc1</chem>
Mol. weight [g/mol]:	160.26
CAS:	1746-23-2

Physical Properties

Property code	Value	Unit	Source
gf	243.62	kJ/mol	Joback Method
hf	50.73	kJ/mol	Joback Method
hfus	11.79	kJ/mol	Joback Method
hvap	43.28	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.627		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
tb	499.07	K	Joback Method
tc	717.29	K	Joback Method
tf	264.60	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.81	J/molxK	499.07	Joback Method
cpg	406.23	J/molxK	680.92	Joback Method
cpg	393.17	J/molxK	644.55	Joback Method
cpg	379.17	J/molxK	608.18	Joback Method

cpg	364.15	J/molxK	571.81	Joback Method
cpg	348.05	J/molxK	535.44	Joback Method
cpg	418.39	J/molxK	717.29	Joback Method
dvisc	0.0001958	Paxs	499.07	Joback Method
dvisc	0.0002570	Paxs	459.99	Joback Method
dvisc	0.0003548	Paxs	420.91	Joback Method
dvisc	0.0005233	Paxs	381.84	Joback Method
dvisc	0.0008432	Paxs	342.76	Joback Method
dvisc	0.0015363	Paxs	303.68	Joback Method
dvisc	0.0033417	Paxs	264.60	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40653e+01
Coeff. B	-4.00725e+03
Coeff. C	-8.01500e+01
Temperature range (K), min.	371.00
Temperature range (K), max.	537.92

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1746232&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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