

Benzene, 1,3-diethenyl-

Other names:	1,3-Diethenylbenzene 1,3-Divinylbenzene Benzene, m-divinyl- Divinylbenzene m-Divinylbenzene m-Vinylstyrene
Inchi:	InChI=1S/C10H10/c1-3-9-6-5-7-10(4-2)8-9/h3-8H,1-2H2
InchiKey:	PRJNEUBECVAVAG-UHFFFAOYSA-N
Formula:	C10H10
SMILES:	C=Cc1cccc(C=C)c1
Mol. weight [g/mol]:	130.19
CAS:	108-57-6

Physical Properties

Property code	Value	Unit	Source
gf	311.78	kJ/mol	Joback Method
hf	226.19	kJ/mol	Joback Method
hfus	12.75	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.973		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
rinpol	1091.30		NIST Webbook
rinpol	1085.20		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	184.20		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	184.20		NIST Webbook
rinpol	1091.30		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1084.80		NIST Webbook
rinpol	1091.00		NIST Webbook
ripol	1541.00		NIST Webbook
ripol	1541.00		NIST Webbook

ripol	1541.00		NIST Webbook
tb	453.22	K	Joback Method
tc	668.56	K	Joback Method
tf	220.90 ± 0.05	K	NIST Webbook
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.07	J/mol×K	453.22	Joback Method
cpg	237.39	J/mol×K	489.11	Joback Method
cpg	249.89	J/mol×K	525.00	Joback Method
cpg	261.61	J/mol×K	560.89	Joback Method
cpg	272.58	J/mol×K	596.78	Joback Method
cpg	282.84	J/mol×K	632.67	Joback Method
cpg	292.44	J/mol×K	668.56	Joback Method
dvisc	0.0019528	Pa×s	237.88	Joback Method
dvisc	0.0010628	Pa×s	273.77	Joback Method
dvisc	0.0006660	Pa×s	309.66	Joback Method
dvisc	0.0004599	Pa×s	345.55	Joback Method
dvisc	0.0003405	Pa×s	381.44	Joback Method
dvisc	0.0002655	Pa×s	417.33	Joback Method
dvisc	0.0002153	Pa×s	453.22	Joback Method
hvapt	48.30	kJ/mol	379.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	325.20	K	0.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$

Coeff. A	1.69595e+01
Coeff. B	-4.94851e+03
Coeff. C	-4.80710e+01
Temperature range (K), min.	344.89
Temperature range (K), max.	472.91

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108576&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Diffusion coefficients of 2-fluoroanisole, 2-bromoanisole, anisole and 1,3-divinylbenzene at infinite dilution in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2007.07.039
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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