trans-«beta»-Methylstyrene

Other names:	(E)- «beta»-Methylstyrene
	trans-Propenylbenzene
	Benzene, 1-propenyl-, (E)-
	(E)-1-Propenyl benzene
Inchi:	InChI=1S/C9H10/c1-2-6-9-7-4-3-5-8-9/h2-8H,1H3/b6-2+
InchiKey:	QROGIFZRVHSFLM-QHHAFSJGSA-N
Formula:	C9H10
SMILES:	CC=Cc1ccccc1
Mol. weight [g/mol]:	118.18
CAS:	873-66-5

Physical Properties

Property code	Value	Unit	Source
affp	834.20	kJ/mol	NIST Webbook
basg	805.30	kJ/mol	NIST Webbook
chg	-5087.95	kJ/mol	NIST Webbook
chl	-4985.20	kJ/mol	NIST Webbook
gf	217.53	kJ/mol	Joback Method
hf	124.66	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	37.86	kJ/mol	Joback Method
ie	8.34	eV	NIST Webbook
ie	8.32	eV	NIST Webbook
ie	8.20 ± 0.02	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	7.84 ± 0.04	eV	NIST Webbook
log10ws	-2.71		Crippen Method
logp	2.720		Crippen Method
mcvol	109.610	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1019.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1009.90		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1008.00		NIST Webbook
ripol	1390.30		NIST Webbook
ripol	1423.60		NIST Webbook

ripol	1364.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1423.60		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1430.10		NIST Webbook
ripol	1390.30		NIST Webbook
tb	450.15 ± 1.50	K	NIST Webbook
tb	447.65 ± 4.00	K	NIST Webbook
tb	451.23 ± 0.40	K	NIST Webbook
tb	449.95 ± 1.50	K	NIST Webbook
tb	451.41 ± 0.30	K	NIST Webbook
tb	449.15 ± 2.00	K	NIST Webbook
tb	448.20	K	NIST Webbook
tc	654.10	K	Joback Method
tf	246.65 ± 1.00	K	NIST Webbook
tf	243.23 ± 0.20	K	NIST Webbook
tf	243.82 ± 0.15	K	NIST Webbook
tf	242.15 ± 4.00	K	NIST Webbook
tf	243.08 ± 0.50	K	NIST Webbook
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.03	J/mol×K	436.16	Joback Method
cpg	212.72	J/mol×K	472.48	Joback Method
cpg	225.50	J/mol×K	508.81	Joback Method
cpg	237.43	J/mol×K	545.13	Joback Method
cpg	248.56	J/mol×K	581.46	Joback Method
cpg	258.93	J/mol×K	617.78	Joback Method
cpg	268.59	J/mol×K	654.10	Joback Method
dvisc	0.0032236	Pa×s	212.53	Joback Method
dvisc	0.0014202	Pa×s	249.80	Joback Method
dvisc	0.0007741	Pa×s	287.07	Joback Method
dvisc	0.0004851	Pa×s	324.34	Joback Method
dvisc	0.0003347	Pa×s	361.62	Joback Method
dvisc	0.0002476	Pa×s	398.89	Joback Method
dvisc	0.0001928	Pa×s	436.16	Joback Method
hvapt	46.40	kJ/mol	371.50	NIST Webbook

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=C873665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
chl:	Standard liquid enthalpy of combustion
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume