2,4,6-Trimethylstyrene

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:	C=Cc1c(C)cc(C)cc1C
Mol. weight [g/mol]:	146.23

Physical Properties

Property code	Value	Unit	Source
af	0.4147		Cheméo Relay (1.0)
gf	213.10	kJ/mol	Joback Method
hf	83.83	kJ/mol	Cheméo Relay (1.0)
hfus	15.84	kJ/mol	Joback Method
hvap	54.58	kJ/mol	Cheméo Relay (1.0)
ie	8.33	eV	NIST Webbook
log10ws	-3.79		Cheméo Relay (1.0)
logp	3.255		Crippen Method
mcvol	137.790	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
tb	477.00 ± 5.00	K	NIST Webbook
tb	482.20	K	NIST Webbook
tc	688.87	K	Cheméo Relay (1.0)
tf	236.15 ± 0.50	K	NIST Webbook
vc	0.506	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.52	J/mol×K	664.52	Joback Method

cpg	359.41	J/mol×K	699.55	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	284.33	J/mol×K	489.38	Joback Method
dvisc	0.0005173	Pa×s	347.09	Joback Method
dvisc	0.0007579	Pa×s	311.52	Joback Method
dvisc	0.0012252	Pa×s	275.95	Joback Method
dvisc	0.0003791	Pa×s	382.67	Joback Method
dvisc	0.0002929	Pa×s	418.24	Joback Method
dvisc	0.0002357	Pa×s	453.81	Joback Method
dvisc	0.0001957	Pa×s	489.38	Joback Method
hvapt	50.90	kJ/mol	422.50	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C769255&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
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