

2,4,5-trimethylstyrene

Inchi:	InChI=1S/C11H14/c1-5-11-7-9(3)8(2)6-10(11)4/h5-7H,1H2,2-4H3
InchiKey:	SVGCCRAIYFQZQM-UHFFFAOYSA-N
Formula:	C11H14
SMILES:	C=Cc1cc(C)c(C)cc1C
Mol. weight [g/mol]:	146.23
CAS:	3937-24-4

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
log10ws	-3.72		Crippen Method
logp	3.255		Crippen Method
mcvol	137.790	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
tb	489.38	K	Joback Method
tc	699.55	K	Joback Method
tf	275.65 ± 0.50	K	NIST Webbook
vc	0.524	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.41	J/mol×K	699.55	Joback Method
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
dvisc	0.0001957	Paxs	489.38	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
hvapt	56.40	kJ/mol	421.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52919e+01
Coeff. B	-4.01207e+03
Coeff. C	-9.81350e+01
Temperature range (K), min.	352.00
Temperature range (K), max.	500.13

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

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=C3937244&Units=SI>

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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