Benzene, 2-(1,3-butadienyl)-1,3,5-trimethyl-

Other names:	1,3-Butadiene, 1-mesityl- Mesitylene, 2-(1,3-butadienyl)- 2-[1,3-Butadienyl]-1,3,5-trimethylbenzene 1,3,5-trimethyl-2-(1,3-butadienyl)benzene 1-Mesitylbuta-1,3-diene
Inchi:	InChI=1S/C13H16/c1-5-6-7-13-11(3)8-10(2)9-12(13)4/h5-9H,1H2,2-4H3/b7-6+
InchiKey:	YOPHSFAXJIMOIN-VOTSOKGWSA-N
Formula:	C13H16
SMILES:	C=CC=Cc1c(C)cc(C)cc1C
Mol. weight [g/mol]:	172.27
CAS:	5732-00-3

Physical Properties

Property code	Value	Unit	Source
gf	310.16	kJ/mol	Joback Method
hf	133.12	kJ/mol	Joback Method
hfus	21.22	kJ/mol	Joback Method
hvap	48.08	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.811		Crippen Method
mcvol	161.670	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1373.00		NIST Webbook
rinpol	1373.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1714.00		NIST Webbook
tb	539.30	K	Joback Method
tc	752.61	K	Joback Method
tf	293.41	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	356.77	J/mol×K	539.30	Joback Method
cpg	372.37	J/mol×K	574.85	Joback Method
cpg	387.09	J/mol×K	610.40	Joback Method
cpg	400.98	J/mol×K	645.96	Joback Method
cpg	414.08	J/mol×K	681.51	Joback Method
cpg	426.43	J/mol×K	717.06	Joback Method
cpg	438.09	J/mol×K	752.61	Joback Method
dvisc	0.0012135	Pa×s	293.41	Joback Method
dvisc	0.0006976	Pa×s	334.39	Joback Method
dvisc	0.0004526	Pa×s	375.37	Joback Method
dvisc	0.0003197	Pa×s	416.36	Joback Method
dvisc	0.0002404	Pa×s	457.34	Joback Method
dvisc	0.0001894	Pa×s	498.32	Joback Method
dvisc	0.0001548	Pa×s	539.30	Joback Method

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=C5732003&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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