m-Cymenene

Other names:	1-Methyl-3-(prop-1-en-2-yl)benzene
	1-methyl-3«alpha»-methylstyrene
	1-methyl-3Â«alphaÂ»-methylstyrene
	Benzene, 1-methyl-3-(1-methylethenyl)-
	m,«alpha»-dimethylstyrene
	m,Â«alphaÂ»-dimethylstyrene
Inchi:	InChI=1S/C10H12/c1-8(2)10-6-4-5-9(3)7-10/h4-7H,1H2,2-3H3
InchiKey:	XXTQHVKTTBLFRI-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	C=C(C)c1cccc(C)c1
Mol. weight [g/mol]:	132.20
CAS:	1124-20-5

Physical Properties

Property code	Value	Unit	Source
affp	867.60	kJ/mol	NIST Webbook
basg	838.70	kJ/mol	NIST Webbook
gf	215.39	kJ/mol	Joback Method
hf	90.97	kJ/mol	Joback Method
hfus	12.72	kJ/mol	Joback Method
hvap	40.20	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.028		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	1061.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1084.10		NIST Webbook

rinpol	1061.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1072.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1456.00		NIST Webbook
tb	456.42	K	Joback Method
tc	671.23	K	Joback Method
tf	225.68	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.50	J/mol×K	456.42	Joback Method
cpg	254.75	J/mol×K	492.22	Joback Method
cpg	268.18	J/mol×K	528.02	Joback Method
cpg	280.82	J/mol×K	563.82	Joback Method
cpg	292.71	J/mol×K	599.62	Joback Method
cpg	303.88	J/mol×K	635.42	Joback Method
cpg	314.37	J/mol×K	671.23	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1124205&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol738.mol

Legend

affp: Proton affinity
basg: Gas basicity

cpg:	Ideal gas heat capacity
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