p-Mentha-1,5,8-triene

Other names:	1,5,8-p-Menthatriene
	5-Isopropenyl-2-methyl-cyclohexa-1,3-diene
	1,5,8-Menthatriene
	p-Mentha-l,5,8-triene
	p-Mentha-1,3,8-triene
	p-1,3,8-Menthatriene
	1,3,8-Menthatriene
	1,3,8-para-Menthatriene
	1,5,8-p-Mentatriene
	p-Menta-1,3,8-triene
Inchi:	InChI=1S/C10H14/c1-8(2)10-6-4-9(3)5-7-10/h4-6,10H,1,7H2,2-3H3
InchiKey:	NJLNIOKPXKKALD-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	C=C(C)C1C=CC(C)=CC1
Mol. weight [g/mol]:	134.22
CAS:	21195-59-5

Physical Properties

Property code	Value	Unit	Source
hfus	12.96	kJ/mol	Joback Method
hvap	49.57	kJ/mol	Cheméo Relay (1.0)
logp	3.085		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
rinpol	1127.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1110.00		NIST Webbook

rinpol	1110.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1113.00	NIST Webbook
rinpol	1112.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1123.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1114.00	NIST Webbook
rinpol	1138.50	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1110.00	NIST Webbook
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ripol	1429.00	NIST Webbook
ripol	1453.00	NIST Webbook
ripol	1383.00	NIST Webbook
ripol	1392.00	NIST Webbook
ripol	1408.00	NIST Webbook

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-4.46300e+01
Coeff. B	8.84340e-01
Coeff. C	-5.33920e-04
Coeff. D	1.20100e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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