Cyclohexene, 3-methyl-6-(1-methylethenyl)-, (3R-trans)-

Other names: p-Mentha-2,8-diene, (1R,4R)-(+)-
(+)-(1R,4R)-trans-Isolimonene
(+)-trans-Isolimonene
Isolimonene
Isolimonene, trans-(+)-
(+)-3R-trans-Isolimonene
3-Isopropenyl-6-methyl-1-cyclohexene-, (3R-trans)-
E-isolimonene
3-Isopropenyl-6-methyl-cyclohexene
trans-Isolimonene
(3R-trans)-3-methyl-6-(1-methylvinyl)cyclohexene

Inchi: InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4,6,9-10H,1,5,7H2,2-3H3/t9-,10-/m1/s1

InchiKey: TWCNAXRPQBLSNO-NXEZZACHSA-N

Formula: C10H16

SMILES: C=C(C)C1C=CC(C)CC1

Mol. weight [g/mol]: 136.23

CAS: 5113-87-1

Physical Properties

Property code	Value	Unit	Source
gf	159.31	kJ/mol	Joback Method
hf	-42.33	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	37.68	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.165		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	981.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	998.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	994.00		NIST Webbook

tb	438.80	K	Joback Method
tc	645.73	K	Joback Method
tf	190.64	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.35	J/mol×K	438.80	Joback Method
cpg	286.78	J/mol×K	473.29	Joback Method
cpg	304.27	J/mol×K	507.78	Joback Method
cpg	320.83	J/mol×K	542.27	Joback Method
cpg	336.50	J/mol×K	576.76	Joback Method
cpg	351.31	J/mol×K	611.25	Joback Method
cpg	365.28	J/mol×K	645.73	Joback Method

Sources

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=C5113871&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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