(+)-3-Carene

Other names:	(+)-«delta»3-Carene (1S)-3,7,7-trimethylbicyclo[4.1.0]hept-3-ene (1S,6R)-3,7,7-trimethylbicyclo[4.1.0]hept-3-ene (1S,6R)-3-carene 3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene-, (1S,6R)- Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl-, (1S)- Isodiprene
Inchi:	InChI=1S/C10H16/c1-7-4-5-8-9(6-7)10(8,2)3/h4,8-9H,5-6H2,1-3H3/t8-,9+/m1/s1
InchiKey:	BQOFWKZOCNGFEC-BDAKNGLRSA-N
Formula:	C10H16
SMILES:	CC1=CCC2C(C1)C2(C)C
Mol. weight [g/mol]:	136.23
CAS:	498-15-7

Physical Properties

Property code	Value	Unit	Source
gf	149.85	kJ/mol	Joback Method
hf	-69.08	kJ/mol	Joback Method
hfus	11.43	kJ/mol	Joback Method
hvap	48.50	kJ/mol	NIST Webbook
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	994.21		NIST Webbook
rinpol	1002.83		NIST Webbook
rinpol	1005.88		NIST Webbook
rinpol	1008.96		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1025.31		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	1021.88		NIST Webbook
rinpol	994.21		NIST Webbook
rinpol	1008.96		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1018.60		NIST Webbook

rinpol	1000.00		NIST Webbook
rinpol	1015.29		NIST Webbook
rinpol	996.99		NIST Webbook
rinpol	1012.09		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1012.09		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1148.00		NIST Webbook
tb	442.63	K	Measurement and correlation of vapor-liquid equilibrium data for binary systems composed of camphene, (+)-3-carene, (-)-beta-caryophyllene, p-cymene, and alpha-pinene at 101.33 kPa
tc	654.83	K	Joback Method
tf	267.76	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.36	J/mol×K	445.66	Joback Method
cpg	292.47	J/mol×K	480.52	Joback Method
cpg	309.23	J/mol×K	515.38	Joback Method
cpg	324.78	J/mol×K	550.25	Joback Method
cpg	339.25	J/mol×K	585.11	Joback Method
cpg	352.77	J/mol×K	619.97	Joback Method
cpg	365.49	J/mol×K	654.83	Joback Method
hvapt	42.80	kJ/mol	401.00	NIST Webbook
pvap	101.33	kPa	442.63	Measurement and correlation of vapor-liquid equilibrium data for binary systems composed of camphene, (+)-3-carene, (-)-beta-caryophyllene, p-cymene, and alpha-pinene at 101.33 kPa

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.70	K	26.70	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Measurement and correlation of vapor-liquid equilibrium data for binary systems composed of camphene, (+)-3-carene, (-)-beta-caryophyllene, p-cymene, and alpha-pinene at 101.33 kPa: https://www.doi.org/10.1016/j.tca.2019.178318

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=C498157&Units=SI

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
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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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