

(+)-2-Carene

Other names:	(+)-«delta»-2-carene (+)-Â«deltaÂ»-2-carene
Inchi:	InChI=1S/C10H16/c1-7-4-5-8-9(6-7)10(8,2)3/h6,8-9H,4-5H2,1-3H3
InchiKey:	IBVJWOMJGCHRRW-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	CC1=CC2C(CC1)C2(C)C
Mol. weight [g/mol]:	136.23
CAS:	4497-92-1

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	37.35	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	993.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	988.00		NIST Webbook
ripol	1158.00		NIST Webbook
tb	445.66	K	Joback Method
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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.32527e+01
Coeff. B	-3.21557e+03
Coeff. C	-7.12880e+01
Temperature range (K), min.	298.15
Temperature range (K), max.	476.21

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U149946&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor 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

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