

Carvone oxide

Other names:	trans-Carvone oxide Carvone-1,2-epoxide carvon-1,2-oxide trans-Carvone epoxide 1-methyl-4-(1-methylvinyl)-7-oxabicyclo[4.1.0]heptan-2-one
Inchi:	InChI=1S/C10H14O2/c1-6(2)7-4-8(11)10(3)9(5-7)12-10/h7,9H,1,4-5H2,2-3H3
InchiKey:	YGMNGQDLUQECTO-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	C=C(C)C1CC(=O)C2(C)OC2C1
Mol. weight [g/mol]:	166.22
CAS:	33204-74-9

Physical Properties

Property code	Value	Unit	Source
gf	0.10	kJ/mol	Joback Method
hf	-269.45	kJ/mol	Joback Method
hfus	15.50	kJ/mol	Joback Method
hvap	44.56	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.699		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1279.00		NIST Webbook

ripol	1279.00		NIST Webbook
ripol	1266.00		NIST Webbook
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ripol	1261.00		NIST Webbook
ripol	1277.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1251.00		NIST Webbook
ripol	1280.00		NIST Webbook
ripol	1277.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1805.00		NIST Webbook
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ripol	1856.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1856.00		NIST Webbook
tb	532.85	K	Joback Method
tc	763.26	K	Joback Method
tf	333.55	K	Joback Method
vc	0.508	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.75	J/mol×K	532.85	Joback Method
cpg	353.90	J/mol×K	571.25	Joback Method

cpg	369.88	J/mol×K	609.65	Joback Method
cpg	384.83	J/mol×K	648.05	Joback Method
cpg	398.91	J/mol×K	686.46	Joback Method
cpg	412.27	J/mol×K	724.86	Joback Method
cpg	425.06	J/mol×K	763.26	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=C33204749&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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