

Pinocarvone

Other names:	2(10)-Pinen-3-one 6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptan-3-one «alpha»-Pinocarvone 3-Nopinenone 2(10)-Pinen-3-one, (.+/-.)- Bicyclo[3.1.1]heptan-3-one, 6,6-dimethyl-2-methylene-(±)-2(10)-pinen-3-one
Inchi:	InChI=1S/C10H14O/c1-6-8-4-7(5-9(6)11)10(8,2)3/h7-8H,1,4-5H2,2-3H3
InchiKey:	TZDMGBLPGZXHJI-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	C=C1C(=O)CC2CC1C2(C)C
Mol. weight [g/mol]:	150.22
CAS:	30460-92-5

Physical Properties

Property code	Value	Unit	Source
gf	60.01	kJ/mol	Joback Method
hf	-168.85	kJ/mol	Joback Method
hfus	8.95	kJ/mol	Joback Method
hvap	40.80	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
rinpol	1164.20		NIST Webbook
tb	508.50	K	Joback Method
tc	733.65	K	Joback Method
tf	336.38	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.45	J/mol×K	508.50	Joback Method

cpg	323.35	J/mol×K	546.02	Joback Method
cpg	339.14	J/mol×K	583.55	Joback Method
cpg	353.96	J/mol×K	621.07	Joback Method
cpg	367.92	J/mol×K	658.60	Joback Method
cpg	381.17	J/mol×K	696.12	Joback Method
cpg	393.81	J/mol×K	733.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30460925&Units=SI
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

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

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