Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-, (1«alpha»,2«alpha»,5«alpha»)-

Other names: trans-3-Pinanone
(E)-Pinocamphone
trans-Pinocamphone
Pinocamphone, trans
Pinocamphone
2,6,6-Trimethylbicyclo[3.1.1]heptan-3-one, (1«alpha»,2«alpha»,5«alpha»)-
3-Pinanone
trans-pinocamphone (pinocamphone)
(1«alpha»,2«alpha»,5«alpha»)-2,6,6-trimethylbicyclo[3.1.1]heptan-3-one

Inchi: InChI=1S/C10H16O/c1-6-8-4-7(5-9(6)11)10(8,2)3/h6-8H,4-5H2,1-3H3

InchiKey: MQPHVIPKLRXGDJ-UHFFFAOYSA-N

Formula: C10H16O

SMILES: CC1C(=O)CC2CC1C2(C)C

Mol. weight [g/mol]: 152.23

CAS: 547-60-4

Physical Properties

Property code	Value	Unit	Source
gf	-0.78	kJ/mol	Joback Method
hf	-273.43	kJ/mol	Joback Method
hfus	11.18	kJ/mol	Joback Method
hvap	40.33	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.258		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1170.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1173.00		NIST Webbook

rinpol	1140.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1161.50	NIST Webbook
rinpol	1160.00	NIST Webbook
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ripol	1507.00	NIST Webbook
ripol	1576.00	NIST Webbook
ripol	1515.00	NIST Webbook
ripol	1482.00	NIST Webbook
ripol	1507.00	NIST Webbook
ripol	1578.00	NIST Webbook

tb	504.67	K	Joback Method
tc	727.60	K	Joback Method
tf	318.46	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.94	J/mol×K	504.67	Joback Method
cpg	343.76	J/mol×K	541.83	Joback Method
cpg	361.40	J/mol×K	578.98	Joback Method
cpg	377.96	J/mol×K	616.14	Joback Method
cpg	393.57	J/mol×K	653.29	Joback Method
cpg	408.36	J/mol×K	690.45	Joback Method
cpg	422.45	J/mol×K	727.60	Joback Method

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=C547604&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume