3-Pinanone

Other names:	(1«alpha»,2«alpha»,5«alpha»)-2,6,6-trimethylbicyclo[3.1.1]heptan-3-one (E)-Pinocamphone 2,6,6-Trimethylbicyclo[3.1.1]heptan-3-one, (1«alpha»,2«alpha»,5«alpha»)- 3-Pinanone Pinocamphone Pinocamphone, trans trans-3-Pinanone trans-Pinocamphone trans-pinocamphone (pinocamphone)
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]:	152.24

Physical Properties

Property code	Value	Unit	Source
hf	-215.96	kJ/mol	Cheméo Relay (1.0)
hfus	11.18	kJ/mol	Joback Method
ie	9.10	eV	Cheméo Relay (1.0)
logp	2.258		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
tb	461.55	K	Cheméo Relay (1.0)
tf	415.52	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C18358537
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point