

trans-Menthone lactone

Inchi: InChI=1S/C10H14O2/c1-6-3-4-9-8(5-6)7(2)10(11)12-9/h6,9H,3-5H2,1-2H3/t6-,9-/m0/s1
InchiKey: DHNNPZQURVIBFL-RCOVLWMOSA-N
Formula: C10H14O2
SMILES: CC1=C2CC(C)CCC2OC1=O
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	-79.49	kJ/mol	Joback Method
hf	-357.47	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	48.57	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.048		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
ripol	1972.00		NIST Webbook
tb	558.38	K	Joback Method
tc	791.07	K	Joback Method
tf	348.37	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.43	J/mol×K	558.38	Joback Method
cpg	355.83	J/mol×K	597.16	Joback Method
cpg	372.24	J/mol×K	635.94	Joback Method
cpg	387.67	J/mol×K	674.73	Joback Method
cpg	402.16	J/mol×K	713.51	Joback Method
cpg	415.71	J/mol×K	752.29	Joback Method
cpg	428.34	J/mol×K	791.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326333&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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