Menthenal isomer

Inchi: InChI=1S/C10H16O/c1-8-3-5-10(6-4-8)9(2)7-11/h7,9-10H,1,3-6H2,2H3
InchiKey: JNRATHVXQNNAQX-UHFFFAOYSA-N
Formula: C10H16O
SMILES: C=C1CCC(C(C)C=O)CC1
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	8.89	kJ/mol	Joback Method
hf	-202.03	kJ/mol	Joback Method
hfus	11.10	kJ/mol	Joback Method
hvap	44.77	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1098.00		NIST Webbook
tb	495.13	K	Joback Method
tc	703.60	K	Joback Method
tf	250.52	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.64	J/mol×K	495.13	Joback Method
cpg	328.62	J/mol×K	529.88	Joback Method
cpg	344.71	J/mol×K	564.62	Joback Method
cpg	359.93	J/mol×K	599.37	Joback Method
cpg	374.31	J/mol×K	634.11	Joback Method
cpg	387.86	J/mol×K	668.86	Joback Method
cpg	400.60	J/mol×K	703.60	Joback Method

dvisc	0.0056040	Pa×s	250.52	Joback Method
dvisc	0.0024868	Pa×s	291.29	Joback Method
dvisc	0.0013471	Pa×s	332.06	Joback Method
dvisc	0.0008345	Pa×s	372.82	Joback Method
dvisc	0.0005681	Pa×s	413.59	Joback Method
dvisc	0.0004144	Pa×s	454.36	Joback Method
dvisc	0.0003184	Pa×s	495.13	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=R224876&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
dvisc:	Dynamic viscosity
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