3-Oxo-p-menth-1-en-7-al

Inchi: InChI=1S/C10H14O2/c1-7(2)9-4-3-8(6-11)5-10(9)12/h5-7,9H,3-4H2,1-2H3
InchiKey: BUAQHWMVENOIOI-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC(C)C1CCC(C=O)=CC1=O
Mol. weight [g/mol]: 166.22
CAS: 160152-34-1

Physical Properties

Property code	Value	Unit	Source
gf	-146.45	kJ/mol	Joback Method
hf	-377.66	kJ/mol	Joback Method
hfus	12.60	kJ/mol	Joback Method
hvap	49.82	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.747		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	1336.00		NIST Webbook
rinpol	1336.00		NIST Webbook
tb	567.93	K	Joback Method
tc	792.78	K	Joback Method
tf	318.34	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.45	J/mol×K	567.93	Joback Method
cpg	359.63	J/mol×K	605.40	Joback Method
cpg	374.95	J/mol×K	642.88	Joback Method
cpg	389.41	J/mol×K	680.35	Joback Method
cpg	402.98	J/mol×K	717.83	Joback Method
cpg	415.67	J/mol×K	755.30	Joback Method
cpg	427.47	J/mol×K	792.78	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=C160152341&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
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