(E)-4-(3-Oxo-2,6,6-trimethylcyclohex-1-en-1-yl)-3-b

Other names: trans-3-Oxo-«alpha»-ionol
Inchi: InChI=1S/C13H20O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h5-7,10,12,14H,8H2,1-4H3
InchiKey: MDCGEAGEQVMWPE-AATRIKPKSA-N
Formula: C13H20O2
SMILES: CC1=CC(=O)CC(C)(C)C1C=CC(C)O
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-91.47	kJ/mol	Joback Method
hf	-394.11	kJ/mol	Joback Method
hfus	17.14	kJ/mol	Joback Method
hvap	64.95	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.485		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	1661.00		NIST Webbook
rinpol	1661.00		NIST Webbook
ripol	2659.00		NIST Webbook
ripol	2659.00		NIST Webbook
tb	679.82	K	Joback Method
tc	891.27	K	Joback Method
tf	385.55	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.02	J/mol×K	679.82	Joback Method
cpg	529.35	J/mol×K	715.06	Joback Method
cpg	544.95	J/mol×K	750.30	Joback Method
cpg	559.91	J/mol×K	785.55	Joback Method
cpg	574.32	J/mol×K	820.79	Joback Method

cpg	588.28	J/mol×K	856.03	Joback Method
cpg	601.88	J/mol×K	891.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R423320&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

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