(Z)-2,2-Dimethyl-3-(3-methylpenta-2,4-dien-1-yl)ox

Inchi: InChI=1S/C10H16O/c1-5-8(2)6-7-9-10(3,4)11-9/h5-6,9H,1,7H2,2-4H3/b8-6-
InchiKey: LIMXJCIGROLRED-VURMDHGXSA-N
Formula: C10H16O
SMILES: C=CC(C)=CCC1OC1(C)C
Mol. weight [g/mol]: 152.23
CAS: 33281-83-3

Physical Properties

Property code	Value	Unit	Source
gf	154.26	kJ/mol	Joback Method
hf	-81.17	kJ/mol	Joback Method
hfus	20.15	kJ/mol	Joback Method
hvap	40.19	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.686		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1133.10		NIST Webbook
rinpol	1133.10		NIST Webbook
tb	458.18	K	Joback Method
tc	657.47	K	Joback Method
tf	245.83	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.19	J/mol×K	458.18	Joback Method
cpg	318.21	J/mol×K	491.40	Joback Method
cpg	333.07	J/mol×K	524.61	Joback Method
cpg	346.90	J/mol×K	557.83	Joback Method
cpg	359.80	J/mol×K	591.04	Joback Method
cpg	371.90	J/mol×K	624.26	Joback Method
cpg	383.32	J/mol×K	657.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33281833&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume