«beta»-Ionyl acetate

Other names: 3-(2,6,6-trimethyl-1-cyclohexen-1-yl)propen-1-yl acetate
Inchi: InChI=1S/C15H24O2/c1-11-7-6-10-15(4,5)14(11)9-8-12(2)17-13(3)16/h8-9,12H,6-7,10H2
InchiKey: WODKSVNXBYBTQC-CMDGGOBGSA-N
Formula: C15H24O2
SMILES: CC(=O)OC(C)C=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 236.35
CAS: 22030-19-9

Physical Properties

Property code	Value	Unit	Source
gf	-51.06	kJ/mol	Joback Method
hf	-381.39	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	58.60	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.021		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	651.52	K	Joback Method
tc	865.00	K	Joback Method
tf	367.97	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.90	J/mol×K	651.52	Joback Method
cpg	587.72	J/mol×K	687.10	Joback Method
cpg	605.60	J/mol×K	722.68	Joback Method
cpg	622.67	J/mol×K	758.26	Joback Method
cpg	639.04	J/mol×K	793.84	Joback Method

cpg	654.81	J/mol×K	829.42	Joback Method
cpg	670.10	J/mol×K	865.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22030199&Units=SI

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