6-(isopropyl)-3-methylcyclohex-2-en-1-yl acetate

Other names: Piperityl acetate
Inchi: InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h7-8,11-12H,5-6H2,1-4H3
InchiKey: NADGBBLSBLDJEH-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CC(=O)OC1C=C(C)CCC1C(C)C
Mol. weight [g/mol]: 196.29
CAS: 1204-30-4

Physical Properties

Property code	Value	Unit	Source
gf	-149.13	kJ/mol	Joback Method
hf	-460.80	kJ/mol	Joback Method
hfus	19.84	kJ/mol	Joback Method
hvap	52.15	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.930		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	1303.30		NIST Webbook
ripol	1900.00		NIST Webbook
tb	568.83	K	Joback Method
tc	775.12	K	Joback Method
tf	298.58	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.48	J/mol×K	568.83	Joback Method
cpg	455.12	J/mol×K	603.21	Joback Method
cpg	472.81	J/mol×K	637.59	Joback Method
cpg	489.57	J/mol×K	671.97	Joback Method
cpg	505.41	J/mol×K	706.36	Joback Method
cpg	520.32	J/mol×K	740.74	Joback Method

cpg	534.32	J/mol×K	775.12	Joback Method
dvisc	0.0025980	Pa×s	298.58	Joback Method
dvisc	0.0013006	Pa×s	343.62	Joback Method
dvisc	0.0007644	Pa×s	388.66	Joback Method
dvisc	0.0005017	Pa×s	433.71	Joback Method
dvisc	0.0003564	Pa×s	478.75	Joback Method
dvisc	0.0002685	Pa×s	523.79	Joback Method
dvisc	0.0002116	Pa×s	568.83	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1204304&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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume