cis-Piperitol, acetate

Other names: cis-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/t1
InchiKey: NADGBBLSBLDJEH-VXGBXAGGSA-N
Formula: C12H20O2
SMILES: CC(=O)OC1C=C(C)CCC1C(C)C
Mol. weight [g/mol]: 196.29
CAS: 112028-22-5

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	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1303.00		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	520.32	J/mol×K	740.74	Joback Method
cpg	505.41	J/mol×K	706.36	Joback Method
cpg	489.57	J/mol×K	671.97	Joback Method
cpg	472.81	J/mol×K	637.59	Joback Method
cpg	455.12	J/mol×K	603.21	Joback Method
cpg	534.32	J/mol×K	775.12	Joback Method
dvisc	0.0002116	Pa×s	568.83	Joback Method
dvisc	0.0002685	Pa×s	523.79	Joback Method
dvisc	0.0003564	Pa×s	478.75	Joback Method
dvisc	0.0005017	Pa×s	433.71	Joback Method
dvisc	0.0007644	Pa×s	388.66	Joback Method
dvisc	0.0013006	Pa×s	343.62	Joback Method
dvisc	0.0025980	Pa×s	298.58	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=C112028225&Units=SI

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume