

Pinchotene acetate

Inchi:	InChI=1S/C12H16O3/c1-8-6-5-7-11(14-4)12(8)9(2)15-10(3)13/h5-7,9H,1-4H3
InchiKey:	TYUGBSLUIRGYKC-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	<chem>COc1cccc(C)c1C(C)OC(C)=O</chem>
Mol. weight [g/mol]:	208.25

Physical Properties

Property code	Value	Unit	Source
gf	-198.05	kJ/mol	Joback Method
hf	-459.72	kJ/mol	Joback Method
hfus	20.55	kJ/mol	Joback Method
hvap	57.08	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.628		Crippen Method
mvol	169.490	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
tb	608.87	K	Joback Method
tc	818.83	K	Joback Method
tf	355.85	K	Joback Method
vc	0.635	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.24	J/molxK	608.87	Joback Method
cpg	434.01	J/molxK	643.86	Joback Method
cpg	448.01	J/molxK	678.86	Joback Method
cpg	461.25	J/molxK	713.85	Joback Method
cpg	473.72	J/molxK	748.85	Joback Method
cpg	485.41	J/molxK	783.84	Joback Method
cpg	496.34	J/molxK	818.83	Joback Method
dvisc	0.0012230	Paxs	355.85	Joback Method

dvisc	0.0006947	Paxs	398.02	Joback Method
dvisc	0.0004398	Paxs	440.19	Joback Method
dvisc	0.0003016	Paxs	482.36	Joback Method
dvisc	0.0002198	Paxs	524.53	Joback Method
dvisc	0.0001678	Paxs	566.70	Joback Method
dvisc	0.0001331	Paxs	608.87	Joback Method

Sources

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=R568879&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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