Pinocarvyl acetate

Other names: trans-Pinocarveyl acetate
trans-Pinocarveol, acetate
(E)-Pinocarvyl acetate
Inchi: InChI=1S/C12H18O2/c1-7-10-5-9(12(10,3)4)6-11(7)14-8(2)13/h9-11H,1,5-6H2,2-4H3
InchiKey: UDBAGFUFASPUFS-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: C=C1C(OC(C)=O)CC2CC1C2(C)C
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	-42.19	kJ/mol	Joback Method
hf	-337.57	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	49.85	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	1281.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1297.00		NIST Webbook

rinpol	1281.00	NIST Webbook
rinpol	1298.00	NIST Webbook
rinpol	1298.00	NIST Webbook
rinpol	1298.00	NIST Webbook
rinpol	1297.00	NIST Webbook
rinpol	1328.00	NIST Webbook
rinpol	1297.00	NIST Webbook
rinpol	1302.30	NIST Webbook
rinpol	1299.00	NIST Webbook
rinpol	1299.00	NIST Webbook
rinpol	1305.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1297.00	NIST Webbook
rinpol	1293.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1296.30	NIST Webbook
rinpol	1266.00	NIST Webbook
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ripol	1661.00	NIST Webbook
ripol	1638.00	NIST Webbook
ripol	1641.00	NIST Webbook
ripol	1657.00	NIST Webbook
ripol	1638.00	NIST Webbook
ripol	1648.00	NIST Webbook
ripol	1681.00	NIST Webbook

ripol	1682.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1681.00		NIST Webbook
ripol	1662.00		NIST Webbook
tb	558.06	K	Joback Method
tc	767.19	K	Joback Method
tf	358.62	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.91	J/mol×K	558.06	Joback Method
cpg	436.52	J/mol×K	592.92	Joback Method
cpg	453.10	J/mol×K	627.77	Joback Method
cpg	468.76	J/mol×K	662.63	Joback Method
cpg	483.62	J/mol×K	697.48	Joback Method
cpg	497.79	J/mol×K	732.34	Joback Method
cpg	511.38	J/mol×K	767.19	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=C1686153&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume