

trans-Pinocarvyl formate

Inchi: InChI=1S/C11H16O2/c1-7-9-4-8(11(9,2)3)5-10(7)13-6-12/h6,8-10H,1,4-5H2,2-3H3
InchiKey: WMHHHHLDOCHBEV-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: C=C1C(OC=O)CC2CC1C2(C)C
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	-21.21	kJ/mol	Joback Method
hf	-289.93	kJ/mol	Joback Method
hfus	16.58	kJ/mol	Joback Method
hvap	47.60	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.150		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1212.00		NIST Webbook
tb	529.97	K	Joback Method
tc	737.39	K	Joback Method
tf	339.42	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.07	J/mol×K	529.97	Joback Method
cpg	387.70	J/mol×K	564.54	Joback Method
cpg	403.32	J/mol×K	599.11	Joback Method
cpg	418.02	J/mol×K	633.68	Joback Method
cpg	431.92	J/mol×K	668.25	Joback Method
cpg	445.12	J/mol×K	702.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R233246&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

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