

trans-Linalool oxide (pyranoid)

Inchi:	InChI=1S/C10H18O2/c1-5-10(4)7-6-8(11)9(2,3)12-10/h5,8,11H,1,6-7H2,2-4H3/t8-,10-/m0
InchiKey:	BCTBAGTXFYWYMW-WPRPVWTQSA-N
Formula:	C10H18O2
SMILES:	C=CC1(C)CCC(O)C(C)(C)O1
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-103.73	kJ/mol	Joback Method
hf	-364.41	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	55.88	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.881		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1176.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1179.00		NIST Webbook
tb	554.70	K	Joback Method
tc	757.96	K	Joback Method
tf	334.79	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.60	J/molxK	554.70	Joback Method
cpg	397.07	J/molxK	588.58	Joback Method
cpg	411.62	J/molxK	622.45	Joback Method
cpg	425.40	J/molxK	656.33	Joback Method
cpg	438.57	J/molxK	690.21	Joback Method
cpg	451.29	J/molxK	724.08	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=R613855&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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