

Androencecalinol

Inchi:	InChI=1S/C12H12O2/c1-3-9-7-10-5-4-6-14-12(10)8-11(9)13-2/h3-5,7-8H,1,6H2,2H3
InchiKey:	NQHVGEQCFZFRTI-UHFFFAOYSA-N
Formula:	C12H12O2
SMILES:	<chem>C=Cc1cc2c(cc1OC)OCC=C2</chem>
Mol. weight [g/mol]:	188.22

Physical Properties

Property code	Value	Unit	Source
gf	116.72	kJ/mol	Joback Method
hf	-82.92	kJ/mol	Joback Method
hfus	23.78	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.744		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	576.47	K	Joback Method
tc	805.20	K	Joback Method
tf	355.44	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.88	J/molxK	576.47	Joback Method
cpg	363.21	J/molxK	614.59	Joback Method
cpg	376.61	J/molxK	652.71	Joback Method
cpg	389.13	J/molxK	690.83	Joback Method
cpg	400.82	J/molxK	728.95	Joback Method
cpg	411.71	J/molxK	767.08	Joback Method
cpg	421.87	J/molxK	805.20	Joback Method
dvisc	0.0012649	Paxs	355.44	Joback Method
dvisc	0.0008616	Paxs	392.28	Joback Method
dvisc	0.0006269	Paxs	429.12	Joback Method

dvisc	0.0004796	Paxs	465.96	Joback Method
dvisc	0.0003817	Paxs	502.79	Joback Method
dvisc	0.0003133	Paxs	539.63	Joback Method
dvisc	0.0002638	Paxs	576.47	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=R341372&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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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