

Cnidilide

Inchi:	InChI=1S/C12H18O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h5,7,9-11H,2-4,6,8H2,1H3
InchiKey:	UXDIXFDKSPCUIX-OUAUKWLOSA-N
Formula:	C12H18O2
SMILES:	CCCCC1OC(=O)C2C=CCCC12
Mol. weight [g/mol]:	194.27
CAS:	3674-03-1

Physical Properties

Property code	Value	Unit	Source
gf	-51.10	kJ/mol	Joback Method
hf	-396.15	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	51.39	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.684		Crippen Method
mvol	161.360	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1700.00		NIST Webbook
tb	589.51	K	Joback Method
tc	811.43	K	Joback Method
tf	341.63	K	Joback Method
vc	0.611	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.67	J/molxK	589.51	Joback Method
cpg	458.40	J/molxK	626.50	Joback Method
cpg	476.97	J/molxK	663.48	Joback Method
cpg	494.40	J/molxK	700.47	Joback Method
cpg	510.72	J/molxK	737.46	Joback Method
cpg	525.97	J/molxK	774.44	Joback Method
cpg	540.16	J/molxK	811.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3674031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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