11-nor-Cadin-5-en-4-one, isomer B

Inchi: InChI=1S/C14H20O/c1-4-11-6-5-10(3)14-12(11)7-9(2)8-13(14)15/h7,11-12H,4-6,8H2,1-3
InchiKey: ABEATVHGSAOQMK-JHJMLUEUSA-N
Formula: C14H20O
SMILES: CCC1CCC(C)=C2C(=O)CC(C)=CC21
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	48.54	kJ/mol	Joback Method
hf	-267.88	kJ/mol	Joback Method
hfus	20.67	kJ/mol	Joback Method
hvap	54.09	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.658		Crippen Method
mcvol	179.370	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
tb	631.36	K	Joback Method
tc	859.92	K	Joback Method
tf	376.64	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.63	J/mol×K	631.36	Joback Method
cpg	508.80	J/mol×K	669.45	Joback Method
cpg	527.77	J/mol×K	707.55	Joback Method
cpg	545.56	J/mol×K	745.64	Joback Method
cpg	562.20	J/mol×K	783.73	Joback Method
cpg	577.70	J/mol×K	821.83	Joback Method
cpg	592.07	J/mol×K	859.92	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=R197130&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume