15-nor-3-Gymnomitrone

Other names: nor-3-Gymnomitrone
Inchi: InChI=1S/C14H22O/c1-12-8-5-11(15)10(9-12)13(2)6-4-7-14(12,13)3/h10H,4-9H2,1-3H3/
InchiKey: VLWAAPCZYHOYCB-VWPFFFCUSA-N
Formula: C14H22O
SMILES: CC12CCC(=O)C(C1)C1(C)CCCC21C
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	78.28	kJ/mol	Joback Method
hf	-238.53	kJ/mol	Joback Method
hfus	3.91	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.572		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1653.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1653.00		NIST Webbook
tb	612.35	K	Joback Method
tc	862.61	K	Joback Method
tf	430.00	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.56	J/mol×K	612.35	Joback Method
cpg	529.66	J/mol×K	654.06	Joback Method
cpg	550.53	J/mol×K	695.77	Joback Method
cpg	570.66	J/mol×K	737.48	Joback Method
cpg	590.55	J/mol×K	779.19	Joback Method
cpg	610.71	J/mol×K	820.90	Joback Method

cpg	631.63	J/mol×K	862.61	Joback Method

Sources

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=R424987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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