cis-14-nor-Muurol-5-en-4-one

Inchi: InChI=1S/C14H22O/c1-9(2)12-6-4-10(3)13-7-5-11(15)8-14(12)13/h8-10,12-13H,4-7H2,1-
InchiKey: AQNMVDGKNNYAEW-WCFLWFBJSA-N
Formula: C14H22O
SMILES: CC(C)C1CCC(C)C2CCC(=O)C=C12
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	27.69	kJ/mol	Joback Method
hf	-328.34	kJ/mol	Joback Method
hfus	17.78	kJ/mol	Joback Method
hvap	51.78	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.594		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1695.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1689.00		NIST Webbook
tb	617.13	K	Joback Method
tc	846.53	K	Joback Method
tf	331.60	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.90	J/mol×K	617.13	Joback Method

cpg	534.67	J/mol×K	655.36	Joback Method
cpg	556.06	J/mol×K	693.60	Joback Method
cpg	576.08	J/mol×K	731.83	Joback Method
cpg	594.76	J/mol×K	770.06	Joback Method
cpg	612.12	J/mol×K	808.30	Joback Method
cpg	628.19	J/mol×K	846.53	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=R411228&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