Muurol-5-en-4-one (cis-14)

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-RTXFEEFZSA-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	1688.00		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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R417855&Units=SI

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