6-«beta»-Hydroxy noreudesman-4-one

Inchi: InChI=1S/C14H24O2/c1-9(2)10-6-8-14(3)7-4-5-11(15)12(14)13(10)16/h9-10,12-13,16H,4
InchiKey: HUHFIOUWECMWGK-SAXRGWBVSA-N
Formula: C14H24O2
SMILES: CC(C)C1CCC2(C)CCCC(=O)C2C1O
Mol. weight [g/mol]: 224.34

Physical Properties

Property code	Value	Unit	Source
gf	-142.66	kJ/mol	Joback Method
hf	-531.98	kJ/mol	Joback Method
hfus	15.81	kJ/mol	Joback Method
hvap	66.04	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.789		Crippen Method
mcvol	193.840	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
ripol	2356.00		NIST Webbook
ripol	2356.00		NIST Webbook
tb	700.74	K	Joback Method
tc	917.59	K	Joback Method
tf	398.80	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.71	J/mol×K	700.74	Joback Method
cpg	624.74	J/mol×K	736.88	Joback Method
cpg	643.77	J/mol×K	773.02	Joback Method
cpg	661.91	J/mol×K	809.16	Joback Method
cpg	679.26	J/mol×K	845.31	Joback Method
cpg	695.94	J/mol×K	881.45	Joback Method
cpg	712.04	J/mol×K	917.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R561254&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume