13-nor-Opposit-4(15)-en-11-one

Inchi: InChI=1S/C14H22O/c1-10-5-4-7-14(3)8-6-12(13(10)14)9-11(2)15/h12-13H,1,4-9H2,2-3H
InchiKey: LTLLRSRCWUAIJT-RUXDESIVSA-N
Formula: C14H22O
SMILES: C=C1CCCC2(C)CCC(CC(C)=O)C12
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	63.16	kJ/mol	Joback Method
hf	-238.61	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	52.55	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.738		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1507.00		NIST Webbook
rinpol	1505.00		NIST Webbook
ripol	2030.00		NIST Webbook
tb	594.61	K	Joback Method
tc	813.60	K	Joback Method
tf	356.13	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.13	J/mol×K	594.61	Joback Method
cpg	514.69	J/mol×K	631.11	Joback Method
cpg	534.02	J/mol×K	667.61	Joback Method
cpg	552.24	J/mol×K	704.10	Joback Method
cpg	569.52	J/mol×K	740.60	Joback Method
cpg	585.99	J/mol×K	777.10	Joback Method
cpg	601.79	J/mol×K	813.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198693&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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