

Onocerane I (8-«beta»-H, 14-«alpha»-H)

Inchi: InChI=1S/C30H54/c1-21-11-15-25-27(3,4)17-9-19-29(25,7)23(21)13-14-24-22(2)12-16-2

InchiKey: DDGSJGSDLIEJOJ-XWODWJSQSA-N

Formula: C30H54

SMILES: CC1CCC2C(C)(C)CCCC2(C)C1CCC1C(C)CCC2C(C)(C)CCCC12C

Mol. weight [g/mol]: 414.75

Physical Properties

Property code	Value	Unit	Source
gf	279.70	kJ/mol	Joback Method
hf	-481.69	kJ/mol	Joback Method
hfus	30.43	kJ/mol	Joback Method
hvap	76.94	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	9.524		Crippen Method
mcvol	390.120	ml/mol	McGowan Method
pc	867.09	kPa	Joback Method
rinpol	3205.00		NIST Webbook
tb	919.86	K	Joback Method
tc	1154.63	K	Joback Method
tf	541.62	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1481.83	J/mol×K	919.86	Joback Method
cpg	1523.87	J/mol×K	958.99	Joback Method
cpg	1567.37	J/mol×K	998.12	Joback Method
cpg	1612.88	J/mol×K	1037.25	Joback Method
cpg	1660.94	J/mol×K	1076.37	Joback Method
cpg	1712.11	J/mol×K	1115.50	Joback Method
cpg	1766.93	J/mol×K	1154.63	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R215471&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

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