

«beta»-Oplopenone

Other names:	Oplopenone «beta»-Oploplenone
Inchi:	InChI=1S/C15H24O/c1-9(2)12-6-5-10(3)13-7-8-14(11(4)16)15(12)13/h9,12-15H,3,5-8H2
InchiKey:	YKWVCZPTAAKDIY-FGZQJIAISA-N
Formula:	C15H24O
SMILES:	<chem>C=C1CCC(C(C)C)C2C1CCC2C(C)=O</chem>
Mol. weight [g/mol]:	220.35
CAS:	28305-60-4

Physical Properties

Property code	Value	Unit	Source
gf	66.92	kJ/mol	Joback Method
hf	-300.11	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	55.22	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.840		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	1601.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1596.00		NIST Webbook
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rinpol	1606.00	NIST Webbook
rinpol	1592.00	NIST Webbook
rinpol	1606.00	NIST Webbook
rinpol	1600.00	NIST Webbook
rinpol	1601.00	NIST Webbook
rinpol	1607.00	NIST Webbook
rinpol	1606.00	NIST Webbook
rinpol	1606.00	NIST Webbook
rinpol	1606.00	NIST Webbook
rinpol	1606.00	NIST Webbook
rinpol	1586.00	NIST Webbook
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rinpol	1605.00	NIST Webbook
rinpol	1592.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1608.00	NIST Webbook
rinpol	1610.00	NIST Webbook
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rinpol	1600.00	NIST Webbook
rinpol	1606.00	NIST Webbook
rinpol	1606.00	NIST Webbook
rinpol	1593.00	NIST Webbook
rinpol	1594.00	NIST Webbook
rinpol	1607.00	NIST Webbook
rinpol	1620.00	NIST Webbook
rinpol	1592.00	NIST Webbook
rinpol	1608.00	NIST Webbook
rinpol	1575.00	NIST Webbook
rinpol	1608.00	NIST Webbook
rinpol	1607.00	NIST Webbook
rinpol	1590.00	NIST Webbook
rinpol	1597.00	NIST Webbook
rinpol	1608.00	NIST Webbook
rinpol	1611.00	NIST Webbook
rinpol	1573.00	NIST Webbook
rinpol	1606.00	NIST Webbook
ripol	2091.00	NIST Webbook
ripol	2064.00	NIST Webbook
ripol	2089.00	NIST Webbook
ripol	2112.00	NIST Webbook
ripol	2092.00	NIST Webbook
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ripol	2092.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2092.00		NIST Webbook
ripol	2129.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2051.00		NIST Webbook
ripol	2061.00		NIST Webbook
ripol	2073.00		NIST Webbook
tb	612.14	K	Joback Method
tc	823.71	K	Joback Method
tf	324.26	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.92	J/molxK	612.14	Joback Method
cpg	572.89	J/molxK	647.40	Joback Method
cpg	593.57	J/molxK	682.66	Joback Method
cpg	612.99	J/molxK	717.93	Joback Method
cpg	631.20	J/molxK	753.19	Joback Method
cpg	648.26	J/molxK	788.45	Joback Method
cpg	664.21	J/molxK	823.71	Joback Method
dvisc	0.0025848	Paxs	324.26	Joback Method
dvisc	0.0017596	Paxs	372.24	Joback Method
dvisc	0.0013078	Paxs	420.22	Joback Method
dvisc	0.0010329	Paxs	468.20	Joback Method
dvisc	0.0008524	Paxs	516.18	Joback Method
dvisc	0.0007268	Paxs	564.16	Joback Method
dvisc	0.0006354	Paxs	612.14	Joback Method

Sources

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=C28305604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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