«beta»-Oplopenone

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-XQLPTFJDSA-N
Formula: C15H24O
SMILES: C=C1CCC(C(C)C)C2C1CCC2C(C)=O
Mol. weight [g/mol]: 220.35

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	1620.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1607.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1611.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1607.00		NIST Webbook
ripol	2098.00		NIST Webbook
ripol	2098.00		NIST Webbook
ripol	2098.00		NIST Webbook
tb	612.14	K	Joback Method
tc	823.71	K	Joback Method
tf	324.26	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.92	J/mol×K	612.14	Joback Method
cpg	572.89	J/mol×K	647.40	Joback Method
cpg	593.57	J/mol×K	682.66	Joback Method
cpg	612.99	J/mol×K	717.93	Joback Method
cpg	631.20	J/mol×K	753.19	Joback Method
cpg	648.26	J/mol×K	788.45	Joback Method
cpg	664.21	J/mol×K	823.71	Joback Method
dvisc	0.0025848	Pa×s	324.26	Joback Method
dvisc	0.0017596	Pa×s	372.24	Joback Method
dvisc	0.0013078	Pa×s	420.22	Joback Method
dvisc	0.0010329	Pa×s	468.20	Joback Method
dvisc	0.0008524	Pa×s	516.18	Joback Method
dvisc	0.0007268	Pa×s	564.16	Joback Method
dvisc	0.0006354	Pa×s	612.14	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=R600309&Units=SI

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