1-((1S,3aR,4R,7S,7aS)-4-Hydroxy-7-isopropyl-4-m

Other names:	Oplopanone (-)-Oplopanone Oplopanon Ethanone, 1-[(1S,3aR,4R,7S,7aS)-octahydro-4-hydroxy-4-methyl-7-(1-methylethyl)-1H-inden-1-yl]- 10-Hydroxyoplopanone
Inchi:	InChI=1S/C15H26O2/c1-9(2)11-7-8-15(4,17)13-6-5-12(10(3)16)14(11)13/h9,11-14,17H,5
InchiKey:	WLXJHVQYKOJBBN-NJVJYBDUSA-N
Formula:	C15H26O2
SMILES:	CC(=O)C1CCC2C1C(C(C)C)CCC2(C)O
Mol. weight [g/mol]:	238.37
CAS:	1911-78-0

Physical Properties

Property code	Value	Unit	Source
gf	-136.18	kJ/mol	Joback Method
hf	-541.68	kJ/mol	Joback Method
hfus	23.65	kJ/mol	Joback Method
hvap	70.28	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.035		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	1734.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1745.30		NIST Webbook
rinpol	1737.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1716.00		NIST Webbook

rinpol	1718.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1711.00		NIST Webbook
ripol	2545.00		NIST Webbook
tb	700.73	K	Joback Method
tc	904.23	K	Joback Method
tf	391.06	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.37	J/mol×K	700.73	Joback Method
cpg	665.58	J/mol×K	734.65	Joback Method
cpg	683.89	J/mol×K	768.56	Joback Method
cpg	701.40	J/mol×K	802.48	Joback Method
cpg	718.23	J/mol×K	836.40	Joback Method
cpg	734.50	J/mol×K	870.31	Joback Method
cpg	750.32	J/mol×K	904.23	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1911780&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
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