Isolongifolanone

Other names: 1,4-Methanoazulen-2(1H)-one, octahydro-4,8,8,9-tetramethyl-, (1«alpha»,3a«beta»,4«alpha»,8a«beta»,9S*)-
(1«alpha»,3a«beta»,4«alpha»,8a«beta»,9S*)-octahydro-4,8,8,9-tetramethyl-1,4-methano

Inchi: InChI=1S/C15H24O/c1-9-12-11(16)8-10-13(12)14(2,3)6-5-7-15(9,10)4/h9-10,12-13H,5-8

InchiKey: XROGGPRBZBLTOH-COPWDGIASA-N

Formula: C15H24O

SMILES: CC1C2C(=O)CC3C2C(C)(C)CCCC13C

Mol. weight [g/mol]: 220.35

CAS: 14727-47-0

Physical Properties

Property code	Value	Unit	Source
gf	76.77	kJ/mol	Joback Method
hf	-315.09	kJ/mol	Joback Method
hfus	14.94	kJ/mol	Joback Method
hvap	50.08	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.674		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1579.60		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1577.90		NIST Webbook
rinpol	1610.00		NIST Webbook
ripol	2037.40		NIST Webbook
ripol	2072.00		NIST Webbook
ripol	2032.90		NIST Webbook
ripol	2072.00		NIST Webbook
ripol	2032.90		NIST Webbook
tb	625.65	K	Joback Method
tc	861.18	K	Joback Method
tf	408.89	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.07	J/mol×K	625.65	Joback Method
cpg	589.71	J/mol×K	664.90	Joback Method
cpg	612.09	J/mol×K	704.16	Joback Method
cpg	633.49	J/mol×K	743.41	Joback Method
cpg	654.20	J/mol×K	782.67	Joback Method
cpg	674.52	J/mol×K	821.92	Joback Method
cpg	694.73	J/mol×K	861.18	Joback Method

Sources

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=C14727470&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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