Isolongifolene, 4,5,9,10-dehydro-

Inchi: InChI=1S/C15H20/c1-13(2)8-5-6-12-14(3,4)11-7-9-15(12,13)10-11/h5-9,11H,10H2,1-4H3
InchiKey: MOLSSUUBCUMURN-UHFFFAOYSA-N
Formula: C15H20
SMILES: CC1(C)C2=CC=CC(C)(C)C23C=CC1C3
Mol. weight [g/mol]: 200.32
CAS: 156747-45-4

Physical Properties

Property code	Value	Unit	Source
gf	289.54	kJ/mol	Joback Method
hf	40.40	kJ/mol	Joback Method
hfus	10.26	kJ/mol	Joback Method
hvap	46.84	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.111		Crippen Method
mcvol	176.730	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1544.00		NIST Webbook
tb	569.87	K	Joback Method
tc	809.58	K	Joback Method
tf	387.85	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.08	J/mol×K	569.87	Joback Method
cpg	482.00	J/mol×K	609.82	Joback Method
cpg	500.35	J/mol×K	649.77	Joback Method
cpg	517.60	J/mol×K	689.72	Joback Method
cpg	534.24	J/mol×K	729.68	Joback Method
cpg	550.75	J/mol×K	769.63	Joback Method
cpg	567.60	J/mol×K	809.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C156747454&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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