Cycloisolongifolene, 8,9-dehydro-

Other names: Didehydro-cycloisolongifolene
Inchi: InChI=1S/C15H22/c1-12(2)6-5-7-14-11-8-10(13(14,3)4)9-15(11,12)14/h5,7,10-11H,6,8-9
InchiKey: KRRPIPKRJIIGHL-UHFFFAOYSA-N
Formula: C15H22
SMILES: CC1(C)CC=CC23C4CC(CC412)C3(C)C
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	323.10	kJ/mol	Joback Method
hf	22.49	kJ/mol	Joback Method
hfus	7.42	kJ/mol	Joback Method
hvap	43.53	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	4.025		Crippen Method
mcvol	174.470	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1311.00		NIST Webbook
tb	556.07	K	Joback Method
tc	791.87	K	Joback Method
tf	421.97	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.26	J/mol×K	556.07	Joback Method
cpg	504.30	J/mol×K	595.37	Joback Method
cpg	523.39	J/mol×K	634.67	Joback Method
cpg	541.17	J/mol×K	673.97	Joback Method
cpg	558.27	J/mol×K	713.27	Joback Method
cpg	575.32	J/mol×K	752.57	Joback Method
cpg	592.96	J/mol×K	791.87	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=U151280&Units=SI

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