(+)-8,9-Didehydrocycloisolongifolene

Inchi: InChI=1S/C15H24/c1-12(2)6-5-7-14-11-8-10(13(14,3)4)9-15(11,12)14/h10-11H,5-9H2,1-
InchiKey: VRSGYUIZSVSWIY-VIQGCOBNSA-N
Formula: C15H24
SMILES: CC1(C)CCCC23C4CC(CC412)C3(C)C
Mol. weight [g/mol]: 204.35
CAS: 74842-33-4

Physical Properties

Property code	Value	Unit	Source
gf	293.14	kJ/mol	Joback Method
hf	-35.29	kJ/mol	Joback Method
hfus	6.20	kJ/mol	Joback Method
hvap	43.24	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.249		Crippen Method
mcvol	178.770	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1321.00		NIST Webbook
rinpol	1321.00		NIST Webbook
tb	556.91	K	Joback Method
tc	790.34	K	Joback Method
tf	421.21	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.47	J/mol×K	556.91	Joback Method
cpg	524.70	J/mol×K	595.81	Joback Method
cpg	544.98	J/mol×K	634.72	Joback Method
cpg	563.90	J/mol×K	673.62	Joback Method
cpg	582.09	J/mol×K	712.53	Joback Method
cpg	600.16	J/mol×K	751.43	Joback Method
cpg	618.71	J/mol×K	790.34	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=C74842334&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