Opposita-4(15),7(11)-dien-1«beta»-ol

Inchi: InChI=1S/C15H24O/c1-10(2)9-12-7-8-15(4)13(16)6-5-11(3)14(12)15/h9,12-14,16H,3,5-8
InchiKey: CZFKRGCIADMIRY-VOFREWHGSA-N
Formula: C15H24O
SMILES: C=C1CCC(O)C2(C)CCC(C=C(C)C)C12
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	127.64	kJ/mol	Joback Method
hf	-211.81	kJ/mol	Joback Method
hfus	22.24	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1636.00		NIST Webbook
ripol	2314.00		NIST Webbook
ripol	2314.00		NIST Webbook
tb	655.17	K	Joback Method
tc	860.33	K	Joback Method
tf	355.01	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.15	J/mol×K	655.17	Joback Method
cpg	590.96	J/mol×K	689.36	Joback Method
cpg	608.83	J/mol×K	723.56	Joback Method
cpg	625.87	J/mol×K	757.75	Joback Method
cpg	642.23	J/mol×K	791.94	Joback Method
cpg	658.03	J/mol×K	826.14	Joback Method

cpg	673.41	J/mol×K	860.33	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=R201284&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume