(E)-Opposita-4(15),7(11)-dien-12-ol

Inchi: InChI=1S/C15H24O/c1-11(10-16)9-13-6-8-15(3)7-4-5-12(2)14(13)15/h9,13-14,16H,2,4-8
InchiKey: AYGVQNVSBUDGKN-BJRRHPIXSA-N
Formula: C15H24O
SMILES: C=C1CCCC2(C)CCC(C=C(C)CO)C12
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	135.35	kJ/mol	Joback Method
hf	-191.47	kJ/mol	Joback Method
hfus	21.17	kJ/mol	Joback Method
hvap	64.74	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1687.00		NIST Webbook
rinpol	1677.00		NIST Webbook
ripol	2428.00		NIST Webbook
tb	659.84	K	Joback Method
tc	865.08	K	Joback Method
tf	359.25	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.29	J/mol×K	659.84	Joback Method
cpg	588.64	J/mol×K	694.05	Joback Method
cpg	606.07	J/mol×K	728.25	Joback Method
cpg	622.71	J/mol×K	762.46	Joback Method
cpg	638.70	J/mol×K	796.67	Joback Method
cpg	654.18	J/mol×K	830.87	Joback Method
cpg	669.28	J/mol×K	865.08	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=R199007&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