(E, E)-3,7,11-Trimethyl-7,10-epoxydodeca-2,5,11-trien

Inchi: InChI=1S/C15H24O2/c1-12(2)14-7-10-15(4,17-14)9-5-6-13(3)8-11-16/h5,8-9,14,16H,1,6-

InchiKey: RHOFVSRBKFWSOJ-OKCSQZJQSA-N

Formula: C15H24O2

SMILES: C=C(C)C1CCC(C)(C=CCC(C)=CCO)O1

Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	107.01	kJ/mol	Joback Method
hf	-241.49	kJ/mol	Joback Method
hfus	31.89	kJ/mol	Joback Method
hvap	68.38	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.385		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1708.00		NIST Webbook
rinpol	1708.00		NIST Webbook
tb	677.34	K	Joback Method
tc	875.96	K	Joback Method
tf	336.92	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.31	J/mol×K	677.34	Joback Method
cpg	610.94	J/mol×K	710.44	Joback Method
cpg	626.80	J/mol×K	743.55	Joback Method
cpg	642.05	J/mol×K	776.65	Joback Method
cpg	656.80	J/mol×K	809.76	Joback Method
cpg	671.19	J/mol×K	842.86	Joback Method
cpg	685.33	J/mol×K	875.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R227360&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

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