Elema-1,11-dien-15-al, epimer a

Inchi: InChI=1S/C15H24O/c1-6-15(5)8-7-13(11(2)3)9-14(15)12(4)10-16/h6,10,12-14H,1-2,7-9H
InchiKey: DFDSCTULEHLJOC-DKUMPPAJSA-N
Formula: C15H24O
SMILES: C=CC1(C)CCC(C(=C)C)CC1C(C)C=O
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	144.13	kJ/mol	Joback Method
hf	-173.84	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	52.72	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	4.006		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	1551.00		NIST Webbook
tb	594.51	K	Joback Method
tc	805.19	K	Joback Method
tf	291.13	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.89	J/mol×K	594.51	Joback Method
cpg	560.94	J/mol×K	629.62	Joback Method
cpg	580.79	J/mol×K	664.74	Joback Method
cpg	599.56	J/mol×K	699.85	Joback Method
cpg	617.38	J/mol×K	734.96	Joback Method
cpg	634.35	J/mol×K	770.07	Joback Method
cpg	650.59	J/mol×K	805.19	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=R397909&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