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

Inchi: InChI=1S/C15H22O/c1-11(10-16)9-13-6-8-15(3)7-4-5-12(2)14(13)15/h9-10,13-14H,2,4-8
InchiKey: DNBAZHCMMBVLFT-BJRRHPIXSA-N
Formula: C15H22O
SMILES: C=C1CCCC2(C)CCC(C=C(C)C=O)C12
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	172.65	kJ/mol	Joback Method
hf	-124.82	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	54.78	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1707.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1679.00		NIST Webbook
ripol	2265.00		NIST Webbook
tb	616.32	K	Joback Method
tc	839.57	K	Joback Method
tf	340.43	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.25	J/mol×K	616.32	Joback Method
cpg	546.67	J/mol×K	653.53	Joback Method
cpg	565.84	J/mol×K	690.74	Joback Method
cpg	583.94	J/mol×K	727.94	Joback Method
cpg	601.14	J/mol×K	765.15	Joback Method

cpg	617.60	J/mol×K	802.36	Joback Method
cpg	633.52	J/mol×K	839.57	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=R198995&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