thujopsenal

Inchi: InChI=1S/C15H24O/c1-13(2)6-4-7-14(3)8-5-11(10-16)12-9-15(12,13)14/h10-12H,4-9H2,1
InchiKey: KTAIRICWMMIGKL-ZJPTYJIISA-N
Formula: C15H24O
SMILES: CC1(C)CCCC2(C)CCC(C=O)C3CC312
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	102.06	kJ/mol	Joback Method
hf	-227.39	kJ/mol	Joback Method
hfus	10.35	kJ/mol	Joback Method
hvap	51.72	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.818		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
ripol	2332.00		NIST Webbook
ripol	2332.00		NIST Webbook
tb	611.40	K	Joback Method
tc	844.94	K	Joback Method
tf	410.81	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.63	J/mol×K	611.40	Joback Method
cpg	571.36	J/mol×K	650.32	Joback Method
cpg	591.82	J/mol×K	689.25	Joback Method
cpg	611.46	J/mol×K	728.17	Joback Method
cpg	630.70	J/mol×K	767.10	Joback Method
cpg	649.98	J/mol×K	806.02	Joback Method
cpg	669.76	J/mol×K	844.94	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=R338955&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume