

Thujopsa-3-one

Inchi: InChI=1S/C15H24O/c1-10-11-8-15(11)13(2,3)6-5-7-14(15,4)9-12(10)16/h10-11H,5-9H2,
InchiKey: LFWRAJWJODKLTN-YIKOMLBNSA-N
Formula: C15H24O
SMILES: CC1C(=O)CC2(C)CCCC(C)(C)C23CC13
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	78.99	kJ/mol	Joback Method
hf	-279.51	kJ/mol	Joback Method
hfus	7.57	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.818		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinsol	1645.00		NIST Webbook
tb	630.56	K	Joback Method
tc	875.45	K	Joback Method
tf	437.03	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.94	J/mol×K	630.56	Joback Method
cpg	584.99	J/mol×K	671.37	Joback Method
cpg	606.96	J/mol×K	712.19	Joback Method
cpg	628.30	J/mol×K	753.00	Joback Method
cpg	649.46	J/mol×K	793.82	Joback Method
cpg	670.93	J/mol×K	834.63	Joback Method
cpg	693.14	J/mol×K	875.45	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=R626801&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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