3-thujopsanone

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,5-9H2,1
InchiKey: LFWRAJWJODKLTN-YIKOMLBNSA-N
Formula: C15H24O
SMILES: CC1C(=O)CC2(C)CCCC(C)(C)C23CC13
Mol. weight [g/mol]: 220.36

Physical Properties

Property code	Value	Unit	Source
hfus	7.57	kJ/mol	Joback Method
logp	3.818		Crippen Method
mcvol	191.200	ml/mol	McGowan 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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25966794&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume