3-iso-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-OGECIDPKSA-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
hfus	7.57	kJ/mol	Joback Method
logp	3.818		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
rinpol	1596.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1620.00		NIST Webbook

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R199874&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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