«beta»-Thujenal

Inchi: InChI=1S/C10H14O/c1-7(2)10-4-3-8(6-11)9(10)5-10/h3-4,6-9H,5H2,1-2H3
InchiKey: UQLNHDYBGCTZNJ-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC(C)C12C=CC(C=O)C1C2
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
hfus	12.69	kJ/mol	Joback Method
logp	2.034		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
rinpol	1195.00		NIST Webbook
rinpol	1195.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.22	J/mol×K	484.63	Joback Method
cpg	315.15	J/mol×K	519.61	Joback Method
cpg	329.80	J/mol×K	554.60	Joback Method
cpg	343.33	J/mol×K	589.58	Joback Method
cpg	355.89	J/mol×K	624.56	Joback Method
cpg	367.61	J/mol×K	659.55	Joback Method
cpg	378.65	J/mol×K	694.53	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R626118&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
Cheméo Relay (1.0):	

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