«alpha»-Thujamenthone

Inchi: InChI=1S/C9H16O/c1-6(2)8-4-5-9(10)7(8)3/h6-8H,4-5H2,1-3H3
InchiKey: VWBCFESGRRREEF-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC(C)C1CCC(=O)C1C
Mol. weight [g/mol]: 140.22

Physical Properties

Property code	Value	Unit	Source
hfus	10.06	kJ/mol	Joback Method
ie	9.15	eV	Cheméo Relay (1.0)
logp	2.258		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
rinpol	1152.00		NIST Webbook
rinpol	1152.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.27	J/mol×K	483.31	Joback Method
cpg	310.04	J/mol×K	518.89	Joback Method
cpg	327.03	J/mol×K	554.48	Joback Method
cpg	343.24	J/mol×K	590.06	Joback Method
cpg	358.67	J/mol×K	625.64	Joback Method
cpg	373.31	J/mol×K	661.23	Joback Method
cpg	387.18	J/mol×K	696.81	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=R324500&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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices