

«delta»-Thujone

Inchi:	InChI=1S/C10H16O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6-8H,4-5H2,1-3H3
InchiKey:	USMNOWBWPHYOEА-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1C(=O)CC2(C(C)C)CC12
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
hfus	8.69	kJ/mol	Joback Method
logp	2.258		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
rinpol	1103.00		NIST Webbook
rinpol	1103.00		NIST Webbook
tb	442.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.27	J/mol×K	504.63	Joback Method
cpg	342.10	J/mol×K	541.27	Joback Method
cpg	358.73	J/mol×K	577.92	Joback Method
cpg	374.30	J/mol×K	614.56	Joback Method
cpg	388.94	J/mol×K	651.20	Joback Method
cpg	402.80	J/mol×K	687.84	Joback Method
cpg	416.01	J/mol×K	724.49	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R516719&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
tb: Normal Boiling Point Temperature

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