«alpha»-Thujamenthol

Inchi: InChI=1S/C10H20O/c1-6(2)9-5-10(11)8(4)7(9)3/h6-11H,5H2,1-4H3
InchiKey: OCXDXSYNPZROSW-UHFFFAOYSA-N
Formula: C10H20O
SMILES: CC(C)C1CC(O)C(C)C1C
Mol. weight [g/mol]: 156.27

Physical Properties

Property code	Value	Unit	Source
hfus	19.37	kJ/mol	Joback Method
hvap	73.84	kJ/mol	Cheméo Relay (1.0)
logp	2.295		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
rinpol	1152.00		NIST Webbook
rinpol	1152.00		NIST Webbook
tb	478.20	K	Cheméo Relay (1.0)
tc	679.90	K	Cheméo Relay (1.0)
tf	315.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.21	J/mol×K	521.21	Joback Method
cpg	461.06	J/mol×K	704.16	Joback Method
cpg	447.67	J/mol×K	673.67	Joback Method
cpg	433.60	J/mol×K	643.18	Joback Method
cpg	418.83	J/mol×K	612.68	Joback Method
cpg	403.35	J/mol×K	582.19	Joback Method
cpg	387.15	J/mol×K	551.70	Joback Method
dvisc	0.0008956	Pa×s	383.84	Joback Method
dvisc	0.0002008	Pa×s	521.21	Joback Method
dvisc	0.0003003	Pa×s	475.42	Joback Method
dvisc	0.0004893	Pa×s	429.63	Joback Method
dvisc	0.0211480	Pa×s	246.46	Joback Method
dvisc	0.0019312	Pa×s	338.04	Joback Method

dvisc	0.0052981	Pa×s	292.25	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R410374&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
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point