

«beta»-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	1174.00		NIST Webbook
rinpol	1174.00		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

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410394&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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