

3-[(E)-1-propenyl]-«alpha»-terpineol P1

Inchi:	InChI=1S/C13H22O/c1-5-6-11-9-10(2)7-8-12(11)13(3,4)14/h5-6,9,11-12,14H,7-8H2,1-4H
InchiKey:	PPYAMQQIEMOEAC-AATRIKPKSA-N
Formula:	C13H22O
SMILES:	CC=CC1C=C(C)CCC1C(C)(C)O
Mol. weight [g/mol]:	194.31

Physical Properties

Property code	Value	Unit	Source
hfus	20.04	kJ/mol	Joback Method
logp	3.306		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
ripol	1803.00		NIST Webbook
ripol	1803.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.21	J/mol×K	608.97	Joback Method
cpg	502.78	J/mol×K	642.26	Joback Method
cpg	519.31	J/mol×K	675.56	Joback Method
cpg	534.86	J/mol×K	708.85	Joback Method
cpg	549.48	J/mol×K	742.14	Joback Method
cpg	563.23	J/mol×K	775.43	Joback Method
cpg	576.15	J/mol×K	808.73	Joback Method
dvisc	0.0097479	Pa×s	310.85	Joback Method
dvisc	0.0023588	Pa×s	360.54	Joback Method
dvisc	0.0008049	Pa×s	410.22	Joback Method
dvisc	0.0003465	Pa×s	459.91	Joback Method
dvisc	0.0001758	Pa×s	509.60	Joback Method
dvisc	0.0001006	Pa×s	559.28	Joback Method
dvisc	0.0000631	Pa×s	608.97	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R327089&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

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