

(1R,3S,4R)-(+)-isomenthol

Inchi:

lnchl=1S/C11H24O/c1-5-7-8-10(9(3)4)11(12)6-2/h9-12H,5-8H2,1-4H3/t10-,11-/m0/s1

InchiKey:

YAJUKXCIXDGILC-QWRGUYRKSA-N

Formula:

C11H24O

SMILES:

CCCCC(C(C)C)C(O)CC

Mol. weight [g/mol]:

172.31

Physical Properties

Property code	Value	Unit	Source
gf	-102.40	kJ/mol	Joback Method
hf	-438.44	kJ/mol	Joback Method
hfus	17.77	kJ/mol	Joback Method
hvap	55.59	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.220		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
ripol	1686.00		NIST Webbook
ripol	1686.00		NIST Webbook
tb	541.94	K	Joback Method
tc	708.25	K	Joback Method
tf	229.55	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.45	J/mol×K	541.94	Joback Method
cpg	444.31	J/mol×K	569.66	Joback Method
cpg	458.56	J/mol×K	597.38	Joback Method
cpg	472.21	J/mol×K	625.09	Joback Method
cpg	485.30	J/mol×K	652.81	Joback Method
cpg	497.82	J/mol×K	680.53	Joback Method
cpg	509.80	J/mol×K	708.25	Joback Method
dvisc	0.2539115	Pa×s	229.55	Joback Method

dvisc	0.0196173	Pa×s	281.62	Joback Method
dvisc	0.0033700	Pa×s	333.68	Joback Method
dvisc	0.0009314	Pa×s	385.75	Joback Method
dvisc	0.0003495	Pa×s	437.81	Joback Method
dvisc	0.0001615	Pa×s	489.87	Joback Method
dvisc	0.0000866	Pa×s	541.94	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R283840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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