Carbonic acid, (1R)-(-)-menthyl isohexyl ester

Inchi: InChI=1S/C17H32O3/c1-12(2)7-6-10-19-17(18)20-16-11-15(13(3)4)9-8-14(16)5/h12-16H
InchiKey: VQUNTWBBGNDWKJ-UHFFFAOYSA-N
Formula: C17H32O3
SMILES: CC(C)CCCOC(=O)OC1CC(C(C)C)CCC1C
Mol. weight [g/mol]: 284.43

Physical Properties

Property code	Value	Unit	Source
gf	-242.51	kJ/mol	Joback Method
hf	-768.15	kJ/mol	Joback Method
hfus	30.69	kJ/mol	Joback Method
hvap	64.04	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	5.037		Crippen Method
mcvol	252.840	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
tb	696.40	K	Joback Method
tc	889.58	K	Joback Method
tf	344.64	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.37	J/mol×K	696.40	Joback Method
cpg	786.11	J/mol×K	728.60	Joback Method
cpg	806.65	J/mol×K	760.79	Joback Method
cpg	825.98	J/mol×K	792.99	Joback Method
cpg	844.12	J/mol×K	825.19	Joback Method
cpg	861.06	J/mol×K	857.38	Joback Method
cpg	876.81	J/mol×K	889.58	Joback Method
dvisc	0.0024258	Pa×s	344.64	Joback Method

dvisc	0.0009978	Pa×s	403.27	Joback Method
dvisc	0.0005142	Pa×s	461.89	Joback Method
dvisc	0.0003077	Pa×s	520.52	Joback Method
dvisc	0.0002043	Pa×s	579.15	Joback Method
dvisc	0.0001462	Pa×s	637.77	Joback Method
dvisc	0.0001107	Pa×s	696.40	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=U392449&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume