

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

Inchi:	InChI=1S/C21H38O3/c1-13(2)17-9-7-15(5)19(11-17)23-21(22)24-20-12-18(14(3)4)10-8-
InchiKey:	FJAKXQSTAVGTSC-UHFFFAOYSA-N
Formula:	C21H38O3
SMILES:	CC(C)C1CCC(C)C(OC(=O)OC2CC(C(C)C)CCC2C)C1
Mol. weight [g/mol]:	338.52

Physical Properties

Property code	Value	Unit	Source
gf	-199.80	kJ/mol	Joback Method
hf	-837.07	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	72.75	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	6.061		Crippen Method
mcvol	298.340	ml/mol	McGowan Method
pc	1180.09	kPa	Joback Method
rinpol	2151.00		NIST Webbook
rinpol	2151.00		NIST Webbook
tb	798.13	K	Joback Method
tc	1008.87	K	Joback Method
tf	388.62	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.83	J/mol×K	798.13	Joback Method
cpg	1115.04	J/mol×K	973.75	Joback Method
cpg	1097.93	J/mol×K	938.63	Joback Method
cpg	1078.95	J/mol×K	903.50	Joback Method
cpg	1058.12	J/mol×K	868.38	Joback Method
cpg	1035.41	J/mol×K	833.25	Joback Method
cpg	1130.30	J/mol×K	1008.87	Joback Method
dvisc	0.0001144	Paxs	798.13	Joback Method

dvisc	0.0001465	Paxs	729.88	Joback Method
dvisc	0.0001975	Paxs	661.63	Joback Method
dvisc	0.0002851	Paxs	593.38	Joback Method
dvisc	0.0004527	Paxs	525.12	Joback Method
dvisc	0.0008255	Paxs	456.87	Joback Method
dvisc	0.0018588	Paxs	388.62	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U392447&Units=SI

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

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