

Carbonic acid, hexadecyl methyl ester

Other names:	Methyl hexadecyl carbonate
Inchi:	InChI=1S/C18H36O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-18(19)20-2/h3-17H2
InchiKey:	WZMKUTXQIPEPTH-UHFFFAOYSA-N
Formula:	C18H36O3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)OC
Mol. weight [g/mol]:	300.48

Physical Properties

Property code	Value	Unit	Source
gf	-238.24	kJ/mol	Joback Method
hf	-791.87	kJ/mol	Joback Method
hfus	46.35	kJ/mol	Joback Method
hvap	67.23	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	6.251		Crippen Method
mvol	277.790	ml/mol	McGowan Method
pc	1175.24	kPa	Joback Method
tb	709.95	K	Joback Method
tc	879.78	K	Joback Method
tf	387.01	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.97	J/molxK	709.95	Joback Method
cpg	906.62	J/molxK	851.47	Joback Method
cpg	891.34	J/molxK	823.17	Joback Method
cpg	875.24	J/molxK	794.86	Joback Method
cpg	858.32	J/molxK	766.56	Joback Method
cpg	840.57	J/molxK	738.25	Joback Method
cpg	921.11	J/molxK	879.78	Joback Method
dvisc	0.0000729	Paxs	709.95	Joback Method
dvisc	0.0000973	Paxs	656.13	Joback Method

dvisc	0.0001367	Paxs	602.30	Joback Method
dvisc	0.0002052	Paxs	548.48	Joback Method
dvisc	0.0003367	Paxs	494.66	Joback Method
dvisc	0.0006234	Paxs	440.83	Joback Method
dvisc	0.0013700	Paxs	387.01	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=U314627&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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