Carbonic acid, methyl octyl ester

Other names: Methyl octyl carbonate
Inchi: InChI=1S/C10H20O3/c1-3-4-5-6-7-8-9-13-10(11)12-2/h3-9H2,1-2H3
InchiKey: MKSDSFWGKQOBHN-UHFFFAOYSA-N
Formula: C10H20O3
SMILES: CCCCCCCCOC(=O)OC
Mol. weight [g/mol]: 188.26

Physical Properties

Property code	Value	Unit	Source
gf	-305.60	kJ/mol	Joback Method
hf	-626.75	kJ/mol	Joback Method
hfus	25.63	kJ/mol	Joback Method
hvap	49.42	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	3.130		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1270.10		NIST Webbook
rinpol	1269.50		NIST Webbook
ripol	1743.40		NIST Webbook
ripol	1744.80		NIST Webbook
ripol	1743.40		NIST Webbook
tb	526.91	K	Joback Method
tc	698.72	K	Joback Method
tf	296.85	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.21	J/mol×K	526.91	Joback Method
cpg	459.09	J/mol×K	670.09	Joback Method
cpg	447.09	J/mol×K	641.45	Joback Method
cpg	434.61	J/mol×K	612.82	Joback Method

cpg	421.63	J/mol×K	584.18	Joback Method
cpg	408.16	J/mol×K	555.55	Joback Method
cpg	470.59	J/mol×K	698.72	Joback Method
dvisc	0.0001822	Pa×s	526.91	Joback Method
dvisc	0.0002362	Pa×s	488.57	Joback Method
dvisc	0.0003200	Pa×s	450.22	Joback Method
dvisc	0.0004589	Pa×s	411.88	Joback Method
dvisc	0.0007084	Pa×s	373.54	Joback Method
dvisc	0.0012078	Pa×s	335.19	Joback Method
dvisc	0.0023638	Pa×s	296.85	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U314620&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume