

Carbonic acid, ethyl cyclohexylmethyl ester

Inchi:	InChI=1S/C10H18O3/c1-2-12-10(11)13-8-9-6-4-3-5-7-9/h9H,2-8H2,1H3
InchiKey:	SDJYCGZAOAKUKM-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	CCOC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	186.25

Physical Properties

Property code	Value	Unit	Source
gf	-281.15	kJ/mol	Joback Method
hf	-572.43	kJ/mol	Joback Method
hfus	17.47	kJ/mol	Joback Method
hvap	49.85	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.740		Crippen Method
mcvol	154.210	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinsol	1296.00		NIST Webbook
tb	546.46	K	Joback Method
tc	749.89	K	Joback Method
tf	304.23	K	Joback Method
vc	0.571	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.27	J/molxK	546.46	Joback Method
cpg	399.70	J/molxK	580.37	Joback Method
cpg	416.30	J/molxK	614.27	Joback Method
cpg	432.06	J/molxK	648.18	Joback Method
cpg	446.99	J/molxK	682.08	Joback Method
cpg	461.09	J/molxK	715.99	Joback Method
cpg	474.35	J/molxK	749.89	Joback Method
dvisc	0.0029761	Paxs	304.23	Joback Method
dvisc	0.0014503	Paxs	344.60	Joback Method

dvisc	0.0008218	Paxs	384.97	Joback Method
dvisc	0.0005187	Paxs	425.35	Joback Method
dvisc	0.0003545	Paxs	465.72	Joback Method
dvisc	0.0002575	Paxs	506.09	Joback Method
dvisc	0.0001961	Paxs	546.46	Joback Method

Sources

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=U357915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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