

Carbonic acid, propyl cyclohexylmethyl ester

Inchi: InChI=1S/C11H20O3/c1-2-8-13-11(12)14-9-10-6-4-3-5-7-10/h10H,2-9H2,1H3
InchiKey: QJRNAVLRITASNNZ-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: CCCOC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 200.27

Physical Properties

Property code	Value	Unit	Source
gf	-272.73	kJ/mol	Joback Method
hf	-593.07	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	3.130		Crippen Method
mvol	168.300	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1433.00		NIST Webbook
rinpol	1433.00		NIST Webbook
tb	569.34	K	Joback Method
tc	769.82	K	Joback Method
tf	315.50	K	Joback Method
vc	0.626	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.87	J/molxK	569.34	Joback Method
cpg	449.95	J/molxK	602.75	Joback Method
cpg	467.15	J/molxK	636.17	Joback Method
cpg	483.47	J/molxK	669.58	Joback Method
cpg	498.91	J/molxK	702.99	Joback Method
cpg	513.47	J/molxK	736.40	Joback Method
cpg	527.16	J/molxK	769.82	Joback Method
dvisc	0.0028391	Paxs	315.50	Joback Method

dvisc	0.0013616	Paxs	357.81	Joback Method
dvisc	0.0007627	Paxs	400.11	Joback Method
dvisc	0.0004774	Paxs	442.42	Joback Method
dvisc	0.0003242	Paxs	484.73	Joback Method
dvisc	0.0002343	Paxs	527.03	Joback Method
dvisc	0.0001777	Paxs	569.34	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=U357816&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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