

Carbonic acid, propyl 2-pentyl ester

Inchi: InChI=1S/C9H18O3/c1-4-6-8(3)12-9(10)11-7-5-2/h8H,4-7H2,1-3H3
InchiKey: VAHDWZIMSOLTCA-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: CCCOC(=O)OC(C)CCC
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
gf	-316.46	kJ/mol	Joback Method
hf	-611.39	kJ/mol	Joback Method
hfus	19.52	kJ/mol	Joback Method
hvap	46.81	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.738		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1109.00		NIST Webbook
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tb	503.59	K	Joback Method
tc	680.25	K	Joback Method
tf	270.58	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.25	J/molxK	503.59	Joback Method
cpg	361.64	J/molxK	533.03	Joback Method
cpg	374.58	J/molxK	562.48	Joback Method
cpg	387.05	J/molxK	591.92	Joback Method
cpg	399.06	J/molxK	621.36	Joback Method
cpg	410.59	J/molxK	650.81	Joback Method
cpg	421.65	J/molxK	680.25	Joback Method
dvisc	0.0033518	Paxs	270.58	Joback Method

dvisc	0.0015333	Paxs	309.41	Joback Method
dvisc	0.0008351	Paxs	348.25	Joback Method
dvisc	0.0005138	Paxs	387.09	Joback Method
dvisc	0.0003454	Paxs	425.92	Joback Method
dvisc	0.0002481	Paxs	464.75	Joback Method
dvisc	0.0001875	Paxs	503.59	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=U357814&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
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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