

Carbonic acid, octyl prop-1-en-2-yl ester

Inchi:	InChI=1S/C12H22O3/c1-4-5-6-7-8-9-10-14-12(13)15-11(2)3/h2,4-10H2,1,3H3
InchiKey:	NRNVYHXLRVTBKQ-UHFFFAOYSA-N
Formula:	C12H22O3
SMILES:	C=C(C)OC(=O)OCCCCCCCC
Mol. weight [g/mol]:	214.30

Physical Properties

Property code	Value	Unit	Source
gf	-209.47	kJ/mol	Joback Method
hf	-552.39	kJ/mol	Joback Method
hfus	28.22	kJ/mol	Joback Method
hvap	53.28	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.034		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinsol	1407.00		NIST Webbook
tb	569.23	K	Joback Method
tc	744.00	K	Joback Method
tf	303.67	K	Joback Method
vc	0.732	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.38	J/mol×K	569.23	Joback Method
cpg	486.51	J/mol×K	598.36	Joback Method
cpg	501.04	J/mol×K	627.49	Joback Method
cpg	514.97	J/mol×K	656.61	Joback Method
cpg	528.30	J/mol×K	685.74	Joback Method
cpg	541.04	J/mol×K	714.87	Joback Method
cpg	553.20	J/mol×K	744.00	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=U382540&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
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
mccvol:	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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