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

Inchi: InChI=1S/C15H28O3/c1-4-5-6-7-8-9-10-11-12-13-17-15(16)18-14(2)3/h2,4-13H2,1,3H3
InchiKey: AJTXHMVZAVWDOU-UHFFFAOYSA-N
Formula: C15H28O3
SMILES: C=C(C)OC(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 256.38

Physical Properties

Property code	Value	Unit	Source
gf	-184.21	kJ/mol	Joback Method
hf	-614.31	kJ/mol	Joback Method
hfus	35.99	kJ/mol	Joback Method
hvap	59.96	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.204		Crippen Method
mcvol	231.220	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	1696.00		NIST Webbook
rinpol	1696.00		NIST Webbook
tb	637.87	K	Joback Method
tc	809.82	K	Joback Method
tf	337.48	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.00	J/mol×K	637.87	Joback Method
cpg	644.87	J/mol×K	666.53	Joback Method
cpg	661.02	J/mol×K	695.19	Joback Method
cpg	676.45	J/mol×K	723.85	Joback Method
cpg	691.18	J/mol×K	752.50	Joback Method
cpg	705.21	J/mol×K	781.16	Joback Method
cpg	718.55	J/mol×K	809.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382906&Units=SI

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
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