Carbonic acid, but-3-en-1-yl heptyl ester

Inchi: InChI=1S/C12H22O3/c1-3-5-7-8-9-11-15-12(13)14-10-6-4-2/h4H,2-3,5-11H2,1H3
InchiKey: MAINAQRDASKZOW-UHFFFAOYSA-N
Formula: C12H22O3
SMILES: C=CCCOC(=O)OCCCCCCC
Mol. weight [g/mol]: 214.30

Physical Properties

Property code	Value	Unit	Source
gf	-200.92	kJ/mol	Joback Method
hf	-542.60	kJ/mol	Joback Method
hfus	29.53	kJ/mol	Joback Method
hvap	53.20	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.686		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	1433.00		NIST Webbook
tb	569.35	K	Joback Method
tc	741.55	K	Joback Method
tf	317.63	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.60	J/mol×K	569.35	Joback Method
cpg	540.44	J/mol×K	712.85	Joback Method
cpg	527.83	J/mol×K	684.15	Joback Method
cpg	514.64	J/mol×K	655.45	Joback Method
cpg	500.88	J/mol×K	626.75	Joback Method
cpg	486.53	J/mol×K	598.05	Joback Method
cpg	552.48	J/mol×K	741.55	Joback Method
dvisc	0.0001550	Pa×s	569.35	Joback Method
dvisc	0.0002012	Pa×s	527.40	Joback Method

dvisc	0.0002731	Pa×s	485.44	Joback Method
dvisc	0.0003929	Pa×s	443.49	Joback Method
dvisc	0.0006097	Pa×s	401.54	Joback Method
dvisc	0.0010484	Pa×s	359.58	Joback Method
dvisc	0.0020804	Pa×s	317.63	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=U383228&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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