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

Inchi: InChI=1S/C22H42O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-21-25-22(23)24-20-6
InchiKey: IZKMGIHXJFVCKF-UHFFFAOYSA-N
Formula: C22H42O3
SMILES: C=CCCOC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 354.57

Physical Properties

Property code	Value	Unit	Source
gf	-116.72	kJ/mol	Joback Method
hf	-749.00	kJ/mol	Joback Method
hfus	55.43	kJ/mol	Joback Method
hvap	75.46	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	7.587		Crippen Method
mcvol	329.850	ml/mol	McGowan Method
pc	941.52	kPa	Joback Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		NIST Webbook
tb	798.15	K	Joback Method
tc	978.42	K	Joback Method
tf	430.33	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.68	J/mol×K	798.15	Joback Method
cpg	1057.58	J/mol×K	828.19	Joback Method
cpg	1076.42	J/mol×K	858.24	Joback Method
cpg	1094.23	J/mol×K	888.28	Joback Method
cpg	1111.04	J/mol×K	918.33	Joback Method
cpg	1126.87	J/mol×K	948.37	Joback Method
cpg	1141.73	J/mol×K	978.42	Joback Method
dvisc	0.0009012	Pa×s	430.33	Joback Method

dvisc	0.0003995	Pa×s	491.63	Joback Method
dvisc	0.0002121	Pa×s	552.94	Joback Method
dvisc	0.0001278	Pa×s	614.24	Joback Method
dvisc	0.0000844	Pa×s	675.54	Joback Method
dvisc	0.0000597	Pa×s	736.85	Joback Method
dvisc	0.0000446	Pa×s	798.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383238&Units=SI
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

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