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

Inchi: InChI=1S/C21H40O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20-24-21(22)23-19-6-4-2
InchiKey: OTRORGODLHWRCP-UHFFFAOYSA-N
Formula: C21H40O3
SMILES: C=CCCOC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 340.54

Physical Properties

Property code	Value	Unit	Source
gf	-125.14	kJ/mol	Joback Method
hf	-728.36	kJ/mol	Joback Method
hfus	52.84	kJ/mol	Joback Method
hvap	73.24	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	7.197		Crippen Method
mcvol	315.760	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	775.27	K	Joback Method
tc	952.22	K	Joback Method
tf	419.06	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.22	J/mol×K	775.27	Joback Method
cpg	1063.64	J/mol×K	922.72	Joback Method
cpg	1048.05	J/mol×K	893.23	Joback Method
cpg	1031.53	J/mol×K	863.74	Joback Method
cpg	1014.07	J/mol×K	834.25	Joback Method
cpg	995.64	J/mol×K	804.76	Joback Method
cpg	1078.32	J/mol×K	952.22	Joback Method
dvisc	0.0000513	Pa×s	775.27	Joback Method

dvisc	0.0000686	Pa×s	715.90	Joback Method
dvisc	0.0000967	Pa×s	656.53	Joback Method
dvisc	0.0001458	Pa×s	597.16	Joback Method
dvisc	0.0002407	Pa×s	537.80	Joback Method
dvisc	0.0004502	Pa×s	478.43	Joback Method
dvisc	0.0010054	Pa×s	419.06	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=U383237&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

Latest version available from:
https://www.chemeo.com/cid/87-086-1/Carbonic-acid-but-3-en-1-yl-hexadecyl-ester.pdf
Generated by Cheméo on 2024-10-12 06:24:15.850176386 +0000 UTC m=+3295118.487145636.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.