

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

Inchi: InChI=1S/C20H38O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-23-20(21)22-18-6-4-2/h4
InchiKey: RLDBHLGVCSHTCE-UHFFFAOYSA-N
Formula: C20H38O3
SMILES: C=CCCOC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 326.51

Physical Properties

Property code	Value	Unit	Source
gf	-133.56	kJ/mol	Joback Method
hf	-707.72	kJ/mol	Joback Method
hfus	50.25	kJ/mol	Joback Method
hvap	71.01	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.807		Crippen Method
mcvol	301.670	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
tb	752.39	K	Joback Method
tc	926.73	K	Joback Method
tf	407.79	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.61	J/mol×K	752.39	Joback Method
cpg	934.58	J/mol×K	781.45	Joback Method
cpg	952.61	J/mol×K	810.50	Joback Method
cpg	969.74	J/mol×K	839.56	Joback Method
cpg	985.96	J/mol×K	868.62	Joback Method
cpg	1001.31	J/mol×K	897.67	Joback Method
cpg	1015.80	J/mol×K	926.73	Joback Method
dvisc	0.0011166	Pa×s	407.79	Joback Method

dvisc	0.0005053	Pa×s	465.22	Joback Method
dvisc	0.0002722	Pa×s	522.66	Joback Method
dvisc	0.0001658	Pa×s	580.09	Joback Method
dvisc	0.0001104	Pa×s	637.52	Joback Method
dvisc	0.0000786	Pa×s	694.96	Joback Method
dvisc	0.0000590	Pa×s	752.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U383236&Units=SI

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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