Carbonic acid, but-3-yn-1-yl tridecyl ester

Inchi: InChI=1S/C18H32O3/c1-3-5-7-8-9-10-11-12-13-14-15-17-21-18(19)20-16-6-4-2/h2H,3,5-
InchiKey: QEAAAYOSUFXKSP-UHFFFAOYSA-N
Formula: C18H32O3
SMILES: C#CCCOC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 296.44

Physical Properties

Property code	Value	Unit	Source
gf	-15.17	kJ/mol	Joback Method
hf	-499.97	kJ/mol	Joback Method
hfus	49.33	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.474		Crippen Method
mcvol	269.190	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	2039.00		NIST Webbook
rinpol	2039.00		NIST Webbook
tb	700.07	K	Joback Method
tc	874.49	K	Joback Method
tf	433.98	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.61	J/mol×K	700.07	Joback Method
cpg	789.26	J/mol×K	729.14	Joback Method
cpg	806.09	J/mol×K	758.21	Joback Method
cpg	822.12	J/mol×K	787.28	Joback Method
cpg	837.36	J/mol×K	816.35	Joback Method
cpg	851.82	J/mol×K	845.42	Joback Method
cpg	865.52	J/mol×K	874.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383179&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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