

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

Inchi: InChI=1S/C19H36O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-18-22-19(20)21-17-6-4-2/h4H,2
InchiKey: NHTHEFJZSMRTHM-UHFFFAOYSA-N
Formula: C19H36O3
SMILES: C=CCCOC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 312.49

Physical Properties

Property code	Value	Unit	Source
gf	-141.98	kJ/mol	Joback Method
hf	-687.08	kJ/mol	Joback Method
hfus	47.66	kJ/mol	Joback Method
hvap	68.78	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	6.417		Crippen Method
mvol	287.580	ml/mol	McGowan Method
pc	1132.91	kPa	Joback Method
rinpol	2122.00		NIST Webbook
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tb	729.51	K	Joback Method
tc	901.89	K	Joback Method
tf	396.52	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.95	J/molxK	729.51	Joback Method
cpg	874.47	J/molxK	758.24	Joback Method
cpg	892.12	J/molxK	786.97	Joback Method
cpg	908.90	J/molxK	815.70	Joback Method
cpg	924.83	J/molxK	844.43	Joback Method
cpg	939.93	J/molxK	873.16	Joback Method
cpg	954.22	J/molxK	901.89	Joback Method
dvisc	0.0012342	Paxs	396.52	Joback Method

dvisc	0.0005648	Paxs	452.02	Joback Method
dvisc	0.0003066	Paxs	507.52	Joback Method
dvisc	0.0001878	Paxs	563.01	Joback Method
dvisc	0.0001256	Paxs	618.51	Joback Method
dvisc	0.0000897	Paxs	674.01	Joback Method
dvisc	0.0000675	Paxs	729.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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