

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

Inchi: InChI=1S/C23H44O3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-26-23(24)25-2
InchiKey: MUUACHUKCGMDHF-UHFFFAOYSA-N
Formula: C23H44O3
SMILES: C=CCCOC(=O)OCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 368.59

Physical Properties

Property code	Value	Unit	Source
gf	-108.30	kJ/mol	Joback Method
hf	-769.64	kJ/mol	Joback Method
hfus	58.02	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	7.977		Crippen Method
mvol	343.940	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	2512.00		NIST Webbook
rinpol	2512.00		NIST Webbook
tb	821.03	K	Joback Method
tc	1005.40	K	Joback Method
tf	441.60	K	Joback Method
vc	1.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.94	J/molxK	821.03	Joback Method
cpg	1120.34	J/molxK	851.76	Joback Method
cpg	1139.62	J/molxK	882.49	Joback Method
cpg	1157.79	J/molxK	913.21	Joback Method
cpg	1174.90	J/molxK	943.94	Joback Method
cpg	1190.95	J/molxK	974.67	Joback Method
cpg	1206.00	J/molxK	1005.40	Joback Method
dvisc	0.0008045	Paxs	441.60	Joback Method

dvisc	0.0003533	Paxs	504.84	Joback Method
dvisc	0.0001863	Paxs	568.08	Joback Method
dvisc	0.0001117	Paxs	631.32	Joback Method
dvisc	0.0000735	Paxs	694.55	Joback Method
dvisc	0.0000519	Paxs	757.79	Joback Method
dvisc	0.0000386	Paxs	821.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383239&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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