Carbonic acid, hexadecyl prop-1-en-2-yl ester

Inchi: InChI=1S/C20H38O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-20(21)23-19(2)3/h2
InchiKey: NPIONMYPQNAYPB-UHFFFAOYSA-N
Formula: C20H38O3
SMILES: C=C(C)OC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 326.51

Physical Properties

Property code	Value	Unit	Source
gf	-142.11	kJ/mol	Joback Method
hf	-717.51	kJ/mol	Joback Method
hfus	48.94	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	7.154		Crippen Method
mcvol	301.670	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	752.27	K	Joback Method
tc	927.58	K	Joback Method
tf	393.83	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.25	J/mol×K	752.27	Joback Method
cpg	934.31	J/mol×K	781.49	Joback Method
cpg	952.43	J/mol×K	810.71	Joback Method
cpg	969.63	J/mol×K	839.93	Joback Method
cpg	985.93	J/mol×K	869.15	Joback Method
cpg	1001.35	J/mol×K	898.36	Joback Method
cpg	1015.91	J/mol×K	927.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382903&Units=SI

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