2-Propenoic acid, hexadecyl ester

Other names: Hexadecyl acrylate
Inchi: InChI=1S/C19H36O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-19(20)4-2/h4H,2-3,
InchiKey: PZDUWXKXFAIFOR-UHFFFAOYSA-N
Formula: C19H36O2
SMILES: C=CC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 296.49
CAS: 13402-02-3

Physical Properties

Property code	Value	Unit	Source
gf	-36.98	kJ/mol	Joback Method
hf	-554.86	kJ/mol	Joback Method
hfus	46.47	kJ/mol	Joback Method
hvap	66.37	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.197		Crippen Method
mcvol	281.710	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook
ripol	2402.00		NIST Webbook
ripol	2402.00		NIST Webbook
tb	707.09	K	Joback Method
tc	877.73	K	Joback Method
tf	374.29	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.93	J/mol×K	707.09	Joback Method
cpg	842.64	J/mol×K	735.53	Joback Method
cpg	860.49	J/mol×K	763.97	Joback Method
cpg	877.51	J/mol×K	792.41	Joback Method

cpg	893.71	J/mol×K	820.85	Joback Method
cpg	909.12	J/mol×K	849.29	Joback Method
cpg	923.77	J/mol×K	877.73	Joback Method
dvisc	0.0018146	Pa×s	374.29	Joback Method
dvisc	0.0007925	Pa×s	429.76	Joback Method
dvisc	0.0004182	Pa×s	485.22	Joback Method
dvisc	0.0002517	Pa×s	540.69	Joback Method
dvisc	0.0001664	Pa×s	596.16	Joback Method
dvisc	0.0001181	Pa×s	651.62	Joback Method
dvisc	0.0000884	Pa×s	707.09	Joback Method

Sources

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=C13402023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume