Propanoic acid, hexadecyl ester

Other names: 1-Hexadecanol, propanoate
Hexadecyl propionate
propionic acid, hexadecyl ester
Inchi: InChI=1S/C19H38O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-19(20)4-2/h3-18H2
InchiKey: RSRQBSGZMPVCOI-UHFFFAOYSA-N
Formula: C19H38O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)CC
Mol. weight [g/mol]: 298.50
CAS: 6221-96-1

Physical Properties

Property code	Value	Unit	Source
gf	-124.82	kJ/mol	Joback Method
hf	-680.29	kJ/mol	Joback Method
hfus	47.75	kJ/mol	Joback Method
hvap	67.04	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.421		Crippen Method
mcvol	286.010	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	2079.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2081.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2081.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2084.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2370.00		NIST Webbook
ripol	2367.00		NIST Webbook
ripol	2352.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2370.00		NIST Webbook
tb	710.41	K	Joback Method
tc	879.90	K	Joback Method

tf	376.05	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.69	J/mol×K	710.41	Joback Method
cpg	867.91	J/mol×K	738.66	Joback Method
cpg	886.25	J/mol×K	766.91	Joback Method
cpg	903.75	J/mol×K	795.15	Joback Method
cpg	920.41	J/mol×K	823.40	Joback Method
cpg	936.27	J/mol×K	851.65	Joback Method
cpg	951.34	J/mol×K	879.90	Joback Method
dvisc	0.0018384	Pa×s	376.05	Joback Method
dvisc	0.0007881	Pa×s	431.78	Joback Method
dvisc	0.0004101	Pa×s	487.50	Joback Method
dvisc	0.0002440	Pa×s	543.23	Joback Method
dvisc	0.0001599	Pa×s	598.96	Joback Method
dvisc	0.0001126	Pa×s	654.68	Joback Method
dvisc	0.0000838	Pa×s	710.41	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=C6221961&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