2-Heptadecanone-1-ol, acetate

Inchi: InChI=1S/C19H36O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19(21)17-22-18(2)20/h3-17
InchiKey: LSDQENKWCINLBH-UHFFFAOYSA-N
Formula: C19H36O3
SMILES: CCCCCCCCCCCCCCCC(=O)COC(C)=O
Mol. weight [g/mol]: 312.49
CAS: 116296-24-3

Physical Properties

Property code	Value	Unit	Source
gf	-253.74	kJ/mol	Joback Method
hf	-792.87	kJ/mol	Joback Method
hfus	49.35	kJ/mol	Joback Method
hvap	73.79	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.600		Crippen Method
mcvol	287.580	ml/mol	McGowan Method
pc	1162.45	kPa	Joback Method
tb	764.28	K	Joback Method
tc	942.71	K	Joback Method
tf	425.98	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.43	J/mol×K	764.28	Joback Method
cpg	895.45	J/mol×K	794.02	Joback Method
cpg	912.55	J/mol×K	823.76	Joback Method
cpg	928.74	J/mol×K	853.50	Joback Method
cpg	944.06	J/mol×K	883.24	Joback Method
cpg	958.51	J/mol×K	912.98	Joback Method
cpg	972.13	J/mol×K	942.71	Joback Method
dvisc	0.0013667	Pa×s	425.98	Joback Method
dvisc	0.0006490	Pa×s	482.36	Joback Method

dvisc	0.0003602	Pa×s	538.75	Joback Method
dvisc	0.0002235	Pa×s	595.13	Joback Method
dvisc	0.0001506	Pa×s	651.51	Joback Method
dvisc	0.0001081	Pa×s	707.90	Joback Method
dvisc	0.0000815	Pa×s	764.28	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=C116296243&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume