Hexadecanoic acid, 2-methylpropyl ester

Other names: 2-methylpropyl hexadecanoate
isobutyl hexadecanoate
Isobutyl palmitate
Inchi: InChI=1S/C20H40O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(21)22-18-19(2)3/h19H
InchiKey: OJIBJRXMHVZPLV-UHFFFAOYSA-N
Formula: C20H40O2
SMILES: CCCCCCCCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 312.53
CAS: 110-34-9

Physical Properties

Property code	Value	Unit	Source
gf	-118.84	kJ/mol	Joback Method
hf	-706.21	kJ/mol	Joback Method
hfus	46.82	kJ/mol	Joback Method
hvap	68.88	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.667		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2129.00		NIST Webbook
rinpol	2129.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
ripol	2367.00		NIST Webbook
ripol	2367.00		NIST Webbook
tb	732.85	K	Joback Method
tc	905.32	K	Joback Method
tf	372.32	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	908.95	J/mol×K	732.85	Joback Method
cpg	928.77	J/mol×K	761.59	Joback Method
cpg	947.65	J/mol×K	790.34	Joback Method
cpg	965.61	J/mol×K	819.08	Joback Method
cpg	982.69	J/mol×K	847.83	Joback Method
cpg	998.90	J/mol×K	876.57	Joback Method
cpg	1014.26	J/mol×K	905.32	Joback Method
dvisc	0.0021002	Pa×s	372.32	Joback Method
dvisc	0.0007959	Pa×s	432.41	Joback Method
dvisc	0.0003822	Pa×s	492.50	Joback Method
dvisc	0.0002153	Pa×s	552.59	Joback Method
dvisc	0.0001357	Pa×s	612.67	Joback Method
dvisc	0.0000929	Pa×s	672.76	Joback Method
dvisc	0.0000677	Pa×s	732.85	Joback Method

Sources

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=C110349&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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