tridecanoic acid, hexyl ester

Other names: Hexyl tridecanoate
Inchi: InChI=1S/C19H38O2/c1-3-5-7-9-10-11-12-13-14-15-17-19(20)21-18-16-8-6-4-2/h3-18H2
InchiKey: CYOONLPPEGKHED-UHFFFAOYSA-N
Formula: C19H38O2
SMILES: CCCCCCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 298.50
CAS: 75850-88-3

Physical Properties

Property code	Value	Unit	Source
af	0.9406		Cheméo Relay (1.0)
hf	-751.52	kJ/mol	Cheméo Relay (1.0)
hfus	47.75	kJ/mol	Joback Method
hvap	92.32	kJ/mol	Cheméo Relay (1.0)
ie	9.62	eV	Cheméo Relay (1.0)
log10ws	-6.46		Cheméo Relay (1.0)
logp	6.421		Crippen Method
mcvol	286.010	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
tb	586.21	K	Cheméo Relay (1.0)
tc	766.98	K	Cheméo Relay (1.0)
tf	282.18	K	Cheméo Relay (1.0)
vc	1.125	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.69	J/mol×K	710.41	Joback Method
cpg	951.34	J/mol×K	879.90	Joback Method
cpg	936.27	J/mol×K	851.65	Joback Method
cpg	920.41	J/mol×K	823.40	Joback Method
cpg	903.75	J/mol×K	795.15	Joback Method
cpg	886.25	J/mol×K	766.91	Joback Method
cpg	867.91	J/mol×K	738.66	Joback Method

dvisc	0.0002440	Pa×s	543.23	Joback Method
dvisc	0.0000838	Pa×s	710.41	Joback Method
dvisc	0.0001126	Pa×s	654.68	Joback Method
dvisc	0.0001599	Pa×s	598.96	Joback Method
dvisc	0.0018384	Pa×s	376.05	Joback Method
dvisc	0.0004101	Pa×s	487.50	Joback Method
dvisc	0.0007881	Pa×s	431.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75850883&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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