

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)OCCCCC
Mol. weight [g/mol]:	298.50

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
mvol	286.010	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	2062.00		NIST Webbook
rinpol	2062.00		NIST Webbook
tb	710.41	K	Joback Method
tc	879.90	K	Joback Method
tf	376.05	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0018384	Paxs	376.05	Joback Method
dvisc	0.0007881	Paxs	431.78	Joback Method
dvisc	0.0004101	Paxs	487.50	Joback Method
dvisc	0.0002440	Paxs	543.23	Joback Method
dvisc	0.0001599	Paxs	598.96	Joback Method
dvisc	0.0001126	Paxs	654.68	Joback Method
dvisc	0.0000838	Paxs	710.41	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=U405198&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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