

3-Octenoic acid, decyl ester

Inchi:	InChI=1S/C18H34O2/c1-3-5-7-9-10-11-13-15-17-20-18(19)16-14-12-8-6-4-2/h12,14H,3-
InchiKey:	UPBHDAPLISIDMF-WYMLVPIESA-N
Formula:	C18H34O2
SMILES:	CCCCC=CCC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	282.46

Physical Properties

Property code	Value	Unit	Source
gf	-53.02	kJ/mol	Joback Method
hf	-542.43	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	64.78	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.807		Crippen Method
mvol	267.620	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
tb	691.69	K	Joback Method
tc	864.16	K	Joback Method
tf	359.70	K	Joback Method
vc	1.048	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.00	J/molxK	691.69	Joback Method
cpg	786.32	J/molxK	720.43	Joback Method
cpg	803.81	J/molxK	749.18	Joback Method
cpg	820.48	J/molxK	777.92	Joback Method
cpg	836.37	J/molxK	806.67	Joback Method
cpg	851.50	J/molxK	835.41	Joback Method
cpg	865.91	J/molxK	864.16	Joback Method
dvisc	0.0018910	Paxs	359.70	Joback Method

dvisc	0.0007915	Paxs	415.03	Joback Method
dvisc	0.0004066	Paxs	470.36	Joback Method
dvisc	0.0002403	Paxs	525.70	Joback Method
dvisc	0.0001570	Paxs	581.03	Joback Method
dvisc	0.0001105	Paxs	636.36	Joback Method
dvisc	0.0000822	Paxs	691.69	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=U406130&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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