

3-Octenoic acid, tridecyl ester

Inchi:	InChI=1S/C21H40O2/c1-3-5-7-9-10-11-12-13-14-16-18-20-23-21(22)19-17-15-8-6-4-2/h1
InchiKey:	HLKUBPBBKZJDIJ-BMRADRMJSA-N
Formula:	C21H40O2
SMILES:	CCCCC=CCC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]:	324.54

Physical Properties

Property code	Value	Unit	Source
gf	-27.76	kJ/mol	Joback Method
hf	-604.35	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.977		Crippen Method
mvol	309.890	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	760.33	K	Joback Method
tc	936.69	K	Joback Method
tf	393.51	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.68	J/molxK	760.33	Joback Method
cpg	965.24	J/molxK	789.72	Joback Method
cpg	983.86	J/molxK	819.12	Joback Method
cpg	1001.56	J/molxK	848.51	Joback Method
cpg	1018.40	J/molxK	877.90	Joback Method
cpg	1034.38	J/molxK	907.29	Joback Method
cpg	1049.56	J/molxK	936.69	Joback Method
dvisc	0.0013987	Paxs	393.51	Joback Method

dvisc	0.0005689	Paxs	454.65	Joback Method
dvisc	0.0002864	Paxs	515.78	Joback Method
dvisc	0.0001668	Paxs	576.92	Joback Method
dvisc	0.0001077	Paxs	638.06	Joback Method
dvisc	0.0000751	Paxs	699.19	Joback Method
dvisc	0.0000555	Paxs	760.33	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=U406133&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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