

trans-2-undecenoic acid

Inchi:	InChI=1S/C11H20O2/c1-2-3-4-5-6-7-8-9-10-11(12)13/h9-10H,2-8H2,1H3,(H,12,13)/b10-9
InchiKey:	IGBBVTAVILYDIO-MDZDMXLPSA-N
Formula:	C11H20O2
SMILES:	CCCCCCCCC=CC(=O)O
Mol. weight [g/mol]:	184.28
CAS:	15790-94-0

Physical Properties

Property code	Value	Unit	Source
gf	-143.78	kJ/mol	Joback Method
hf	-417.96	kJ/mol	Joback Method
hfus	30.14	kJ/mol	Joback Method
hvap	63.46	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.378		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	601.29	K	Joback Method
tc	773.34	K	Joback Method
tf	319.40	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.85	J/molxK	601.29	Joback Method
cpg	444.49	J/molxK	629.97	Joback Method
cpg	456.54	J/molxK	658.64	Joback Method
cpg	468.04	J/molxK	687.32	Joback Method
cpg	479.01	J/molxK	715.99	Joback Method
cpg	489.47	J/molxK	744.67	Joback Method
cpg	499.44	J/molxK	773.34	Joback Method
dvisc	0.0091541	Paxs	319.40	Joback Method
dvisc	0.0024450	Paxs	366.38	Joback Method

dvisc	0.0008816	Paxs	413.36	Joback Method
dvisc	0.0003915	Paxs	460.34	Joback Method
dvisc	0.0002020	Paxs	507.33	Joback Method
dvisc	0.0001166	Paxs	554.31	Joback Method
dvisc	0.0000734	Paxs	601.29	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=C15790940&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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