

2,5-undecadienal

Inchi:	InChI=1S/C11H18O/c1-2-3-4-5-6-7-8-9-10-11-12/h6-7,9-11H,2-5,8H2,1H3/b7-6+,10-9+
InchiKey:	XCXOPZBEPMNL SI-AVQMFFATSA-N
Formula:	C11H18O
SMILES:	CCCCC=CCC=CC=O
Mol. weight [g/mol]:	166.26

Physical Properties

Property code	Value	Unit	Source
gf	102.66	kJ/mol	Joback Method
hf	-121.51	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	46.72	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.268		Crippen Method
mvol	158.820	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1352.00		NIST Webbook
tb	508.06	K	Joback Method
tc	690.37	K	Joback Method
tf	245.57	K	Joback Method
vc	0.628	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.24	J/molxK	508.06	Joback Method
cpg	418.52	J/molxK	659.99	Joback Method
cpg	406.97	J/molxK	629.60	Joback Method
cpg	394.80	J/molxK	599.22	Joback Method
cpg	381.98	J/molxK	568.83	Joback Method
cpg	368.47	J/molxK	538.45	Joback Method
cpg	429.49	J/molxK	690.37	Joback Method
dvisc	0.0001939	Paxs	508.06	Joback Method
dvisc	0.0002557	Paxs	464.31	Joback Method

dvisc	0.0003571	Paxs	420.56	Joback Method
dvisc	0.0005390	Paxs	376.81	Joback Method
dvisc	0.0009065	Paxs	333.07	Joback Method
dvisc	0.0017841	Paxs	289.32	Joback Method
dvisc	0.0044691	Paxs	245.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R237035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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