

trans-Undec-4-enal

Other names:	(4E)-4-Undecenal (E)-4-Undecenal
Inchi:	InChI=1S/C11H20O/c1-2-3-4-5-6-7-8-9-10-11-12/h7-8,11H,2-6,9-10H2,1H3/b8-7+
InchiKey:	QGNDNDFXCNBMKI-BQYQJAHWSA-N
Formula:	C11H20O
SMILES:	CCCCCCC=CCCC=O
Mol. weight [g/mol]:	168.28
CAS:	68820-35-9

Physical Properties

Property code	Value	Unit	Source
gf	22.44	kJ/mol	Joback Method
hf	-238.73	kJ/mol	Joback Method
hfus	26.74	kJ/mol	Joback Method
hvap	46.76	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.492		Crippen Method
mvol	163.120	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1191.00		NIST Webbook
rinpol	1191.00		NIST Webbook
tb	503.90	K	Joback Method
tc	678.56	K	Joback Method
tf	250.65	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.55	J/molxK	503.90	Joback Method
cpg	386.13	J/molxK	533.01	Joback Method
cpg	400.06	J/molxK	562.12	Joback Method
cpg	413.35	J/molxK	591.23	Joback Method
cpg	426.04	J/molxK	620.34	Joback Method

cpg	438.14	J/molxK	649.45	Joback Method
cpg	449.68	J/molxK	678.56	Joback Method
dvisc	0.0047920	Paxs	250.65	Joback Method
dvisc	0.0020053	Paxs	292.86	Joback Method
dvisc	0.0010451	Paxs	335.07	Joback Method
dvisc	0.0006302	Paxs	377.27	Joback Method
dvisc	0.0004207	Paxs	419.48	Joback Method
dvisc	0.0003024	Paxs	461.69	Joback Method
dvisc	0.0002297	Paxs	503.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68820359&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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