(E)-4,5-epoxy-(E)-2-undecenal

Other names: trans-4,5-epoxy-(E)-undec-2-enal
Inchi: InChI=1S/C11H18O2/c1-2-3-4-5-7-10-11(13-10)8-6-9-12/h6,8-11H,2-5,7H2,1H3/b8-6+/t1
InchiKey: RMXFWTWOCHIUQP-SIPGATMPSA-N
Formula: C11H18O2
SMILES: CCCCCCC1OC1C=CC=O
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-10.64	kJ/mol	Joback Method
hf	-318.27	kJ/mol	Joback Method
hfus	33.92	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.479		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2100.00		NIST Webbook
tb	532.92	K	Joback Method
tc	719.55	K	Joback Method
tf	290.92	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.39	J/mol×K	532.92	Joback Method
cpg	405.63	J/mol×K	564.02	Joback Method
cpg	420.06	J/mol×K	595.13	Joback Method
cpg	433.72	J/mol×K	626.23	Joback Method
cpg	446.66	J/mol×K	657.34	Joback Method

cpg	458.91	J/mol×K	688.44	Joback Method
cpg	470.52	J/mol×K	719.55	Joback Method
dvisc	0.0024902	Pa×s	290.92	Joback Method
dvisc	0.0016535	Pa×s	331.25	Joback Method
dvisc	0.0011999	Pa×s	371.59	Joback Method
dvisc	0.0009272	Pa×s	411.92	Joback Method
dvisc	0.0007502	Pa×s	452.25	Joback Method
dvisc	0.0006284	Pa×s	492.59	Joback Method
dvisc	0.0005407	Pa×s	532.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R237164&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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