

(2E)-cis-4,5-Epoxy-2-decenal

Inchi:	InChI=1S/C12H22O/c1-3-5-6-9-12(4-2)10-7-8-11-13/h7-8,11-12H,3-6,9-10H2,1-2H3/b8-7
InchiKey:	HIWBOMGTTYWHPK-GUOLPTJISA-N
Formula:	C12H22O
SMILES:	CCCCC(CC)CC=CC=O
Mol. weight [g/mol]:	182.30

Physical Properties

Property code	Value	Unit	Source
gf	28.42	kJ/mol	Joback Method
hf	-264.65	kJ/mol	Joback Method
hfus	25.80	kJ/mol	Joback Method
hvap	48.60	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.738		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
ripol	1986.00		NIST Webbook
tb	526.34	K	Joback Method
tc	702.92	K	Joback Method
tf	246.92	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.08	J/molxK	526.34	Joback Method
cpg	434.74	J/molxK	555.77	Joback Method
cpg	449.67	J/molxK	585.20	Joback Method
cpg	463.92	J/molxK	614.63	Joback Method
cpg	477.50	J/molxK	644.06	Joback Method
cpg	490.44	J/molxK	673.49	Joback Method
cpg	502.78	J/molxK	702.92	Joback Method
dvisc	0.0069575	Paxs	246.92	Joback Method
dvisc	0.0024143	Paxs	293.49	Joback Method

dvisc	0.0011195	Paxs	340.06	Joback Method
dvisc	0.0006247	Paxs	386.63	Joback Method
dvisc	0.0003951	Paxs	433.20	Joback Method
dvisc	0.0002732	Paxs	479.77	Joback Method
dvisc	0.0002016	Paxs	526.34	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=R590920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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