

trans-4,5-epoxy-(E)-dodec-2-enal

Other names:	trans-4,5-Epoxy-(E)-2-dodecenal
Inchi:	InChI=1S/C12H20O2/c1-2-3-4-5-6-8-11-12(14-11)9-7-10-13/h7,9-12H,2-6,8H2,1H3/b9-7
InchiKey:	ZYDXKAHTGWQVMS-JONLBCGYSA-N
Formula:	C12H20O2
SMILES:	CCCCCCCC1OC1C=CC=O
Mol. weight [g/mol]:	196.29

Physical Properties

Property code	Value	Unit	Source
gf	-2.22	kJ/mol	Joback Method
hf	-338.91	kJ/mol	Joback Method
hfus	36.51	kJ/mol	Joback Method
hvap	53.10	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.869		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
ripol	2210.00		NIST Webbook
tb	555.80	K	Joback Method
tc	740.37	K	Joback Method
tf	302.19	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.81	J/molxK	555.80	Joback Method
cpg	454.66	J/molxK	586.56	Joback Method
cpg	469.69	J/molxK	617.32	Joback Method
cpg	483.93	J/molxK	648.08	Joback Method
cpg	497.44	J/molxK	678.85	Joback Method
cpg	510.24	J/molxK	709.61	Joback Method

cpg	522.39	J/molxK	740.37	Joback Method
dvisc	0.0026476	Paxs	302.19	Joback Method
dvisc	0.0017128	Paxs	344.46	Joback Method
dvisc	0.0012187	Paxs	386.73	Joback Method
dvisc	0.0009273	Paxs	429.00	Joback Method
dvisc	0.0007410	Paxs	471.26	Joback Method
dvisc	0.0006144	Paxs	513.53	Joback Method
dvisc	0.0005242	Paxs	555.80	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=R237144&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
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

Latest version available from:

<https://www.chemeo.com/cid/48-082-8/trans-4-5-epoxy-E-dodec-2-enal.pdf>

Generated by Cheméo on 2024-04-19 22:19:10.120006344 +0000 UTC m=+15854399.040583657.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.