

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

Other names:	trans-4,5-epoxy-(E)-oct-2-enal
Inchi:	InChI=1S/C8H12O2/c1-2-4-7-8(10-7)5-3-6-9/h3,5-8H,2,4H2,1H3/b5-3+/t7-,8-/m0/s1
InchiKey:	RBBPXMPGIPJSJY-VKTMEOEOSA-N
Formula:	C8H12O2
SMILES:	CCCC1OC1C=CC=O
Mol. weight [g/mol]:	140.18

Physical Properties

Property code	Value	Unit	Source
gf	-35.90	kJ/mol	Joback Method
hf	-256.35	kJ/mol	Joback Method
hfus	26.15	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	1.309		Crippen Method
mvol	115.860	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1181.00		NIST Webbook
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tb	464.28	K	Joback Method
tc	657.51	K	Joback Method
tf	257.11	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.71	J/molxK	464.28	Joback Method
cpg	268.54	J/molxK	496.49	Joback Method
cpg	280.64	J/molxK	528.69	Joback Method
cpg	292.05	J/molxK	560.90	Joback Method
cpg	302.79	J/molxK	593.10	Joback Method
cpg	312.92	J/molxK	625.31	Joback Method
cpg	322.47	J/molxK	657.51	Joback Method

dvisc	0.0018048	Paxs	257.11	Joback Method
dvisc	0.0013099	Paxs	291.64	Joback Method
dvisc	0.0010175	Paxs	326.17	Joback Method
dvisc	0.0008295	Paxs	360.69	Joback Method
dvisc	0.0007009	Paxs	395.22	Joback Method
dvisc	0.0006084	Paxs	429.75	Joback Method
dvisc	0.0005394	Paxs	464.28	Joback Method

Sources

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=R237184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
mvol:	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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