

trans-4,5-epoxy-(E)-2-nonenal

Other names:	(E)-4,5-epoxy-(E)-2-nonenal tr-4,5-Epoxy-(E)-2- nonenal trans-4,5-epoxy-(E)-non-2-enal
Inchi:	InChI=1S/C9H14O2/c1-2-3-5-8-9(11-8)6-4-7-10/h4,6-9H,2-3,5H2,1H3/b6-4+/t8-,9-/m0/s1
InchiKey:	JQNFKXWEJORMGJ-AIZLHNLISA-N
Formula:	C9H14O2
SMILES:	CCCCC1OC1C=CC=O
Mol. weight [g/mol]:	154.21

Physical Properties

Property code	Value	Unit	Source
gf	-27.48	kJ/mol	Joback Method
hf	-276.99	kJ/mol	Joback Method
hfus	28.74	kJ/mol	Joback Method
hvap	46.42	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.699		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1245.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1884.00		NIST Webbook
tb	487.16	K	Joback Method
tc	678.18	K	Joback Method
tf	268.38	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.74	J/mol×K	487.16	Joback Method
cpg	312.48	J/mol×K	519.00	Joback Method
cpg	325.46	J/mol×K	550.83	Joback Method
cpg	337.71	J/mol×K	582.67	Joback Method
cpg	349.28	J/mol×K	614.51	Joback Method
cpg	360.21	J/mol×K	646.34	Joback Method
cpg	370.52	J/mol×K	678.18	Joback Method
dvisc	0.0020626	Paxs	268.38	Joback Method
dvisc	0.0014504	Paxs	304.84	Joback Method
dvisc	0.0010996	Paxs	341.31	Joback Method
dvisc	0.0008794	Paxs	377.77	Joback Method
dvisc	0.0007316	Paxs	414.23	Joback Method
dvisc	0.0006269	Paxs	450.70	Joback Method
dvisc	0.0005499	Paxs	487.16	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R201477&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	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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