

trans-2,3-epoxynonanal

Inchi:	InChI=1S/C9H16O2/c1-2-3-4-5-6-8-9(7-10)11-8/h7-9H,2-6H2,1H3/t8-,9-/m0/s1
InchiKey:	CXWONQXFWHZHPN-IUCAKERBSA-N
Formula:	C9H16O2
SMILES:	CCCCCCC1OC1C=O
Mol. weight [g/mol]:	156.22

Physical Properties

Property code	Value	Unit	Source
gf	-107.70	kJ/mol	Joback Method
hf	-394.21	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	46.46	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.923		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1194.00		NIST Webbook
rinpol	1194.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1653.00		NIST Webbook
tb	483.00	K	Joback Method
tc	665.54	K	Joback Method
tf	273.46	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.62	J/mol×K	483.00	Joback Method
cpg	329.72	J/mol×K	513.42	Joback Method
cpg	343.14	J/mol×K	543.85	Joback Method
cpg	355.90	J/mol×K	574.27	Joback Method
cpg	368.04	J/mol×K	604.70	Joback Method
cpg	379.56	J/mol×K	635.12	Joback Method

cpg	390.52	J/mol×K	665.54	Joback Method
dvisc	0.0023518	Pa×s	273.46	Joback Method
dvisc	0.0016789	Pa×s	308.38	Joback Method
dvisc	0.0012836	Pa×s	343.31	Joback Method
dvisc	0.0010313	Pa×s	378.23	Joback Method
dvisc	0.0008598	Pa×s	413.15	Joback Method
dvisc	0.0007374	Pa×s	448.08	Joback Method
dvisc	0.0006466	Pa×s	483.00	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=R237104&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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