

trans-2,3-epoxyhexanal

Inchi:	InChI=1S/C6H10O2/c1-2-3-5-6(4-7)8-5/h4-6H,2-3H2,1H3/t5-,6-/m0/s1
InchiKey:	JHKVGI0BTDDGMJ-WDSKDSINSA-N
Formula:	C6H10O2
SMILES:	CCCC1OC1C=O
Mol. weight [g/mol]:	114.14

Physical Properties

Property code	Value	Unit	Source
gf	-132.96	kJ/mol	Joback Method
hf	-332.29	kJ/mol	Joback Method
hfus	20.77	kJ/mol	Joback Method
hvap	39.78	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	0.753		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
rinpol	892.00		NIST Webbook
ripol	1340.00		NIST Webbook
tb	414.36	K	Joback Method
tc	602.02	K	Joback Method
tf	239.65	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.27	J/molxK	414.36	Joback Method
cpg	241.05	J/molxK	570.74	Joback Method
cpg	232.12	J/molxK	539.47	Joback Method
cpg	222.70	J/molxK	508.19	Joback Method
cpg	212.77	J/molxK	476.91	Joback Method
cpg	202.30	J/molxK	445.64	Joback Method
cpg	249.50	J/molxK	602.02	Joback Method
dvisc	0.0005738	Paxs	414.36	Joback Method

dvisc	0.0006323	Paxs	385.24	Joback Method
dvisc	0.0007077	Paxs	356.12	Joback Method
dvisc	0.0008083	Paxs	327.00	Joback Method
dvisc	0.0009474	Paxs	297.89	Joback Method
dvisc	0.0011494	Paxs	268.77	Joback Method
dvisc	0.0014615	Paxs	239.65	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R237095&Units=SI

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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