4,5-epoxydec-2-enal

Inchi: InChI=1S/C10H16O2/c1-2-3-4-6-9-10(12-9)7-5-8-11/h5,7-10H,2-4,6H2,1H3/b7-5+
InchiKey: HIOMEXREAUSUBP-FNORWQNLSA-N
Formula: C10H16O2
SMILES: CCCCCC1OC1C=CC=O
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-19.06	kJ/mol	Joback Method
hf	-297.63	kJ/mol	Joback Method
hfus	31.33	kJ/mol	Joback Method
hvap	48.65	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.089		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1376.00		NIST Webbook
rinpol	1376.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2045.00		NIST Webbook
tb	510.04	K	Joback Method
tc	698.84	K	Joback Method
tf	279.65	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.67	J/mol×K	510.04	Joback Method
cpg	408.89	J/mol×K	667.37	Joback Method
cpg	397.26	J/mol×K	635.91	Joback Method
cpg	384.96	J/mol×K	604.44	Joback Method
cpg	371.96	J/mol×K	572.97	Joback Method

cpg	358.21	J/mol×K	541.51	Joback Method
cpg	419.89	J/mol×K	698.84	Joback Method
dvisc	0.0005498	Pa×s	510.04	Joback Method
dvisc	0.0006332	Pa×s	471.64	Joback Method
dvisc	0.0007476	Pa×s	433.24	Joback Method
dvisc	0.0009117	Pa×s	394.84	Joback Method
dvisc	0.0011605	Pa×s	356.45	Joback Method
dvisc	0.0015657	Pa×s	318.05	Joback Method
dvisc	0.0022936	Pa×s	279.65	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=R303954&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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