

4,5-epoxy-2-decenal (isomer B)

Inchi:	InChI=1S/C10H18O2/c1-2-3-4-6-9-10(12-9)7-5-8-11/h8-10H,2-7H2,1H3
InchiKey:	ZMSFXIUDNVVMIZ-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CCCCC1OC1CCC=O
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-99.28	kJ/mol	Joback Method
hf	-414.85	kJ/mol	Joback Method
hfus	31.13	kJ/mol	Joback Method
hvap	48.69	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.313		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
ripol	1990.00		NIST Webbook
ripol	1990.00		NIST Webbook
tb	505.88	K	Joback Method
tc	686.62	K	Joback Method
tf	284.73	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.06	J/mol×K	505.88	Joback Method
cpg	375.96	J/mol×K	536.00	Joback Method
cpg	390.15	J/mol×K	566.13	Joback Method
cpg	403.65	J/mol×K	596.25	Joback Method
cpg	416.49	J/mol×K	626.37	Joback Method
cpg	428.70	J/mol×K	656.49	Joback Method
cpg	440.30	J/mol×K	686.62	Joback Method
dvisc	0.0025988	Pa×s	284.73	Joback Method

dvisc	0.0018032	Pa×s	321.59	Joback Method
dvisc	0.0013488	Pa×s	358.45	Joback Method
dvisc	0.0010650	Pa×s	395.31	Joback Method
dvisc	0.0008756	Pa×s	432.16	Joback Method
dvisc	0.0007423	Pa×s	469.02	Joback Method
dvisc	0.0006446	Pa×s	505.88	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=R325667&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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