

[4,5-2H2]-trans-4,5-Epoxy-(E)-2-decenal

Inchi:	InChI=1S/C10H18O2/c1-2-3-4-6-9-10(12-9)7-5-8-11/h8-10H,2-7H2,1H3/t9-,10-/m1/s1/i9
InchiKey:	ZMSFXIUDNVVMIZ-XKXKDXACSA-N
Formula:	C10H16D2O2
SMILES:	CCCCC1OC1CCC=O
Mol. weight [g/mol]:	172.26

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	1380.00		NIST Webbook
ripol	2011.00		NIST Webbook
ripol	1995.00		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/molxK	505.88	Joback Method
cpg	428.70	J/molxK	656.49	Joback Method
cpg	416.49	J/molxK	626.37	Joback Method
cpg	403.65	J/molxK	596.25	Joback Method
cpg	390.15	J/molxK	566.13	Joback Method
cpg	375.96	J/molxK	536.00	Joback Method
cpg	440.30	J/molxK	686.62	Joback Method

dvisc	0.0006446	Paxs	505.88	Joback Method
dvisc	0.0007423	Paxs	469.02	Joback Method
dvisc	0.0008756	Paxs	432.16	Joback Method
dvisc	0.0010650	Paxs	395.31	Joback Method
dvisc	0.0013488	Paxs	358.45	Joback Method
dvisc	0.0018032	Paxs	321.59	Joback Method
dvisc	0.0025988	Paxs	284.73	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=R396095&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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