

trans-4,5-Epoxy-(E)-2-decenal

Other names:

4,5-epoxy-(E)-2-decenal
(E)-4,5-Epoxy-(E)-2-decenal
trans-4,5-Epoxy-2(E)-decenal
(E)-2-Decenal, 4,5-epoxy
tr-4,5-Epoxy-(E)-dec-2-enal
trans-4,5-epoxy-(E)-dec-2-enal
(E)-4,5-epoxydec-2-enal
trans-4,5-epoxy-(E)-2-decanal
trans-(E)-2-Decenal, 4,5-epoxy
tr-4,5-Epoxy-(E)-2-decenal
trans-4,5-epoxy-(E)-2-decenale
4,5-epoxy-(E)-dec-2-enal
2-Decenal, (E)-, 4,5-(E)-epoxy-

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+/t9-,10-**InchiKey:** HIOMEXREAU SUBP-IUUOVR RDSA-N**Formula:** C10H16O2**SMILES:** CCCCCC1OC1C=CC=O**Mol. weight [g/mol]:** 168.23**CAS:** 134454-31-2

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	1390.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1383.00		NIST Webbook

rinpol	1379.00	NIST Webbook
rinpol	1380.00	NIST Webbook
rinpol	1392.00	NIST Webbook
rinpol	1374.00	NIST Webbook
rinpol	1389.00	NIST Webbook
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ripol	2017.00	NIST Webbook
ripol	2021.00	NIST Webbook
ripol	2010.00	NIST Webbook
ripol	1989.00	NIST Webbook
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ripol	2017.00	NIST Webbook
ripol	1997.00	NIST Webbook
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ripol	2000.00	NIST Webbook
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ripol	2006.00	NIST Webbook
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ripol	2018.00	NIST Webbook
ripol	1979.00	NIST Webbook
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ripol	2007.00	NIST Webbook

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ripol	2017.00	NIST Webbook
ripol	1989.00	NIST Webbook
ripol	2009.00	NIST Webbook
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ripol	2006.00	NIST Webbook
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ripol	1994.00	NIST Webbook
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ripol	2000.00	NIST Webbook
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ripol	1986.00	NIST Webbook
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ripol	2020.00	NIST Webbook
ripol	2017.00	NIST Webbook
ripol	1994.00	NIST Webbook
ripol	1986.00	NIST Webbook
ripol	2006.00	NIST Webbook
ripol	1978.00	NIST Webbook
ripol	1995.00	NIST Webbook
ripol	2000.00	NIST Webbook
ripol	1987.00	NIST Webbook
ripol	2015.00	NIST Webbook

ripol	2021.00		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/molxK	510.04	Joback Method
cpg	358.21	J/molxK	541.51	Joback Method
cpg	371.96	J/molxK	572.97	Joback Method
cpg	384.96	J/molxK	604.44	Joback Method
cpg	397.26	J/molxK	635.91	Joback Method
cpg	408.89	J/molxK	667.37	Joback Method
cpg	419.89	J/molxK	698.84	Joback Method
dvisc	0.0022936	Paxs	279.65	Joback Method
dvisc	0.0015657	Paxs	318.05	Joback Method
dvisc	0.0011605	Paxs	356.45	Joback Method
dvisc	0.0009117	Paxs	394.84	Joback Method
dvisc	0.0007476	Paxs	433.24	Joback Method
dvisc	0.0006332	Paxs	471.64	Joback Method
dvisc	0.0005498	Paxs	510.04	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C134454312&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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