

trans-4,5-epoxy-(E)-hept-2-enal

Inchi:	InChI=1S/C7H10O2/c1-2-6-7(9-6)4-3-5-8/h3-7H,2H2,1H3/b4-3+/t6-,7-/m0/s1
InchiKey:	PGTKHYGKDOAHEN-FWDZIHJBSA-N
Formula:	C7H10O2
SMILES:	CCC1OC1C=CC=O
Mol. weight [g/mol]:	126.15

Physical Properties

Property code	Value	Unit	Source
gf	-44.32	kJ/mol	Joback Method
hf	-235.71	kJ/mol	Joback Method
hfus	23.56	kJ/mol	Joback Method
hvap	41.97	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	0.919		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	1080.00		NIST Webbook
rinpol	1080.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1698.00		NIST Webbook
tb	441.40	K	Joback Method
tc	636.77	K	Joback Method
tf	245.84	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.68	J/molxK	441.40	Joback Method
cpg	267.10	J/molxK	604.21	Joback Method
cpg	257.86	J/molxK	571.65	Joback Method
cpg	248.04	J/molxK	539.09	Joback Method
cpg	237.59	J/molxK	506.52	Joback Method
cpg	226.48	J/molxK	473.96	Joback Method

cpg	275.79	J/molxK	636.77	Joback Method
dvisc	0.0005172	Paxs	441.40	Joback Method
dvisc	0.0005765	Paxs	408.81	Joback Method
dvisc	0.0006550	Paxs	376.21	Joback Method
dvisc	0.0007623	Paxs	343.62	Joback Method
dvisc	0.0009158	Paxs	311.03	Joback Method
dvisc	0.0011486	Paxs	278.43	Joback Method
dvisc	0.0015297	Paxs	245.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R237159&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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