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/mol×K	441.40	Joback Method
cpg	226.48	J/mol×K	473.96	Joback Method
cpg	237.59	J/mol×K	506.52	Joback Method
cpg	248.04	J/mol×K	539.09	Joback Method
cpg	257.86	J/mol×K	571.65	Joback Method
cpg	267.10	J/mol×K	604.21	Joback Method

cpg	275.79	J/mol×K	636.77	Joback Method
dvisc	0.0015297	Pa×s	245.84	Joback Method
dvisc	0.0011486	Pa×s	278.43	Joback Method
dvisc	0.0009158	Pa×s	311.03	Joback Method
dvisc	0.0007623	Pa×s	343.62	Joback Method
dvisc	0.0006550	Pa×s	376.21	Joback Method
dvisc	0.0005765	Pa×s	408.81	Joback Method
dvisc	0.0005172	Pa×s	441.40	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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