[2,3-2H2]-trans-2,3-Epoxyoctanal

Inchi: InChI=1S/C8H14O2/c1-2-3-4-5-7-8(6-9)10-7/h6-8H,2-5H2,1H3/t7-,8-/m1/s1/i7D,8D
InchiKey: YWFUECKBUFORTA-YAZXJRJDSA-N
Formula: C8H12D2O2
SMILES: CCCCCC1OC1C=O
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
gf	-116.12	kJ/mol	Joback Method
hf	-373.57	kJ/mol	Joback Method
hfus	25.95	kJ/mol	Joback Method
hvap	44.24	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.533		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1093.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1542.00		NIST Webbook
tb	460.12	K	Joback Method
tc	644.46	K	Joback Method
tf	262.19	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.10	J/mol×K	460.12	Joback Method
cpg	285.30	J/mol×K	490.84	Joback Method
cpg	297.85	J/mol×K	521.57	Joback Method
cpg	309.78	J/mol×K	552.29	Joback Method
cpg	321.11	J/mol×K	583.02	Joback Method
cpg	331.87	J/mol×K	613.74	Joback Method

cpg	342.08	J/mol×K	644.46	Joback Method
dvisc	0.0020728	Pa×s	262.19	Joback Method
dvisc	0.0015252	Pa×s	295.18	Joback Method
dvisc	0.0011937	Pa×s	328.17	Joback Method
dvisc	0.0009770	Pa×s	361.15	Joback Method
dvisc	0.0008269	Pa×s	394.14	Joback Method
dvisc	0.0007181	Pa×s	427.13	Joback Method
dvisc	0.0006364	Pa×s	460.12	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=R396080&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
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