

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-/m0/s1
InchiKey:	YWFUECKBUFORTA-YUMQZZPRSA-N
Formula:	C8H14O2
SMILES:	CCCCC1OC1C=O
Mol. weight [g/mol]:	142.20

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	1089.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1092.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1547.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R237119&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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