trans-2,3-epoxyheptanal

Inchi: InChI=1S/C7H12O2/c1-2-3-4-6-7(5-8)9-6/h5-7H,2-4H2,1H3/t6-,7-/m0/s1
InchiKey: JSGLRFSEKUNPRD-BQBZGAKWSA-N
Formula: C7H12O2
SMILES: CCCCC1OC1C=O
Mol. weight [g/mol]: 128.17

Physical Properties

Property code	Value	Unit	Source
gf	-124.54	kJ/mol	Joback Method
hf	-352.93	kJ/mol	Joback Method
hfus	23.36	kJ/mol	Joback Method
hvap	42.01	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.143		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	992.00		NIST Webbook
ripol	1446.00		NIST Webbook
ripol	1446.00		NIST Webbook
tb	437.24	K	Joback Method
tc	623.31	K	Joback Method
tf	250.92	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.62	J/mol×K	437.24	Joback Method
cpg	242.79	J/mol×K	468.25	Joback Method
cpg	254.36	J/mol×K	499.26	Joback Method
cpg	265.35	J/mol×K	530.28	Joback Method
cpg	275.78	J/mol×K	561.29	Joback Method
cpg	285.67	J/mol×K	592.30	Joback Method
cpg	295.06	J/mol×K	623.31	Joback Method

dvisc	0.0017719	Pa×s	250.92	Joback Method
dvisc	0.0013465	Pa×s	281.97	Joback Method
dvisc	0.0010805	Pa×s	313.03	Joback Method
dvisc	0.0009022	Pa×s	344.08	Joback Method
dvisc	0.0007762	Pa×s	375.13	Joback Method
dvisc	0.0006833	Pa×s	406.19	Joback Method
dvisc	0.0006125	Pa×s	437.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R237080&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
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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