trans-2,3-epoxydodecanal

Inchi: InChI=1S/C12H22O2/c1-2-3-4-5-6-7-8-9-11-12(10-13)14-11/h10-12H,2-9H2,1H3/t11-,12-
InchiKey: WJEHBSHUBXDAJC-RYUDHWBXSA-N
Formula: C12H22O2
SMILES: CCCCCCCCCC1OC1C=O
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-82.44	kJ/mol	Joback Method
hf	-456.13	kJ/mol	Joback Method
hfus	36.31	kJ/mol	Joback Method
hvap	53.14	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.093		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1500.00		NIST Webbook
ripol	1967.00		NIST Webbook
ripol	1967.00		NIST Webbook
tb	551.64	K	Joback Method
tc	728.98	K	Joback Method
tf	307.27	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.29	J/mol×K	551.64	Joback Method
cpg	473.52	J/mol×K	581.20	Joback Method
cpg	488.97	J/mol×K	610.75	Joback Method
cpg	503.69	J/mol×K	640.31	Joback Method
cpg	517.71	J/mol×K	669.86	Joback Method
cpg	531.05	J/mol×K	699.42	Joback Method
cpg	543.74	J/mol×K	728.98	Joback Method

dvisc	0.0029699	Pa×s	307.27	Joback Method
dvisc	0.0019561	Pa×s	348.00	Joback Method
dvisc	0.0014062	Pa×s	388.73	Joback Method
dvisc	0.0010762	Pa×s	429.45	Joback Method
dvisc	0.0008627	Pa×s	470.18	Joback Method
dvisc	0.0007163	Pa×s	510.91	Joback Method
dvisc	0.0006114	Pa×s	551.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R237075&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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