Heptyl propyl carbonate

Inchi: InChI=1S/C11H22O3/c1-3-5-6-7-8-10-14-11(12)13-9-4-2/h3-10H2,1-2H3
InchiKey: VOIGYUQYURXJCS-UHFFFAOYSA-N
Formula: C11H22O3
SMILES: CCCCCCCOC(=O)OCCC
Mol. weight [g/mol]: 202.29
CAS: 959272-47-0

Physical Properties

Property code	Value	Unit	Source
gf	-297.18	kJ/mol	Joback Method
hf	-647.39	kJ/mol	Joback Method
hfus	28.22	kJ/mol	Joback Method
hvap	51.65	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.520		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
tb	549.79	K	Joback Method
tc	720.36	K	Joback Method
tf	308.12	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.25	J/mol×K	549.79	Joback Method
cpg	510.63	J/mol×K	691.93	Joback Method
cpg	498.03	J/mol×K	663.50	Joback Method
cpg	484.89	J/mol×K	635.08	Joback Method
cpg	471.21	J/mol×K	606.65	Joback Method
cpg	457.00	J/mol×K	578.22	Joback Method
cpg	522.70	J/mol×K	720.36	Joback Method

dvisc	0.0001660	Pa×s	549.79	Joback Method
dvisc	0.0002161	Pa×s	509.51	Joback Method
dvisc	0.0002945	Pa×s	469.23	Joback Method
dvisc	0.0004253	Pa×s	428.95	Joback Method
dvisc	0.0006628	Pa×s	388.68	Joback Method
dvisc	0.0011445	Pa×s	348.40	Joback Method
dvisc	0.0022797	Pa×s	308.12	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C959272470&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume