Ethyl-3, 4-dihydro-2, -h-pyran carboxylate

Other names: 2H-Pyran-2-carboxylic acid, 3,4-dihydro-, ethyl ester
Inchi: InChI=1S/C8H12O3/c1-2-10-8(9)7-5-3-4-6-11-7/h4,6-7H,2-3,5H2,1H3
InchiKey: HXBSUCZDAYLJDO-UHFFFAOYSA-N
Formula: C8H12O3
SMILES: CCOC(=O)C1CCC=CO1
Mol. weight [g/mol]: 156.18
CAS: 83568-11-0

Physical Properties

Property code	Value	Unit	Source
gf	-249.15	kJ/mol	Joback Method
hf	-473.15	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	47.79	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
log10ws	-1.48		Crippen Method
logp	1.242		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	504.39	K	Joback Method
tc	716.76	K	Joback Method
tf	286.79	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.80	J/mol×K	504.39	Joback Method
cpg	291.15	J/mol×K	539.78	Joback Method
cpg	304.76	J/mol×K	575.18	Joback Method
cpg	317.64	J/mol×K	610.57	Joback Method
cpg	329.79	J/mol×K	645.97	Joback Method
cpg	341.23	J/mol×K	681.36	Joback Method
cpg	351.95	J/mol×K	716.76	Joback Method

dvisc	0.0036127	Pa×s	286.79	Joback Method
dvisc	0.0018663	Pa×s	323.06	Joback Method
dvisc	0.0011016	Pa×s	359.32	Joback Method
dvisc	0.0007162	Pa×s	395.59	Joback Method
dvisc	0.0005006	Pa×s	431.86	Joback Method
dvisc	0.0003698	Pa×s	468.12	Joback Method
dvisc	0.0002854	Pa×s	504.39	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=C83568110&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume