Propyl-d1-formate

Inchi: InChI=1S/C4H8O2/c1-4(2)6-3-5/h3-4H,1-2H3/i3D
InchiKey: RMOUBSOVHSONPZ-WFVSFCRTSA-N
Formula: C4H7DO2
SMILES: CC(C)OC=O
Mol. weight [g/mol]: 89.11
CAS: 60703-00-6

Physical Properties

Property code	Value	Unit	Source
gf	-224.16	kJ/mol	Joback Method
hf	-348.97	kJ/mol	Joback Method
hfus	6.07	kJ/mol	Joback Method
hvap	33.24	kJ/mol	Joback Method
log10ws	-0.47		Crippen Method
logp	0.568		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	361.56	K	Joback Method
tc	539.67	K	Joback Method
tf	184.07	K	Joback Method
vc	0.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.99	J/mol×K	361.56	Joback Method
cpg	138.90	J/mol×K	391.25	Joback Method
cpg	145.62	J/mol×K	420.93	Joback Method
cpg	152.16	J/mol×K	450.62	Joback Method
cpg	158.51	J/mol×K	480.30	Joback Method
cpg	164.66	J/mol×K	509.99	Joback Method
cpg	170.62	J/mol×K	539.67	Joback Method
dvisc	0.0044029	Pa×s	184.07	Joback Method
dvisc	0.0020143	Pa×s	213.65	Joback Method

dvisc	0.0011146	Pa×s	243.23	Joback Method
dvisc	0.0007012	Pa×s	272.81	Joback Method
dvisc	0.0004830	Pa×s	302.40	Joback Method
dvisc	0.0003555	Pa×s	331.98	Joback Method
dvisc	0.0002752	Pa×s	361.56	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=C60703006&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
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