Formic acid, 3-ethylpent-3-yl ester

Inchi: InChI=1S/C8H16O2/c1-4-8(5-2,6-3)10-7-9/h7H,4-6H2,1-3H3
InchiKey: FDNBSOFNQQDCAE-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCC(CC)(CC)OC=O
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
gf	-185.20	kJ/mol	Joback Method
hf	-435.00	kJ/mol	Joback Method
hfus	12.54	kJ/mol	Joback Method
hvap	41.24	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.128		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	972.00		NIST Webbook
rinpol	972.00		NIST Webbook
tb	450.29	K	Joback Method
tc	631.49	K	Joback Method
tf	246.57	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.42	J/mol×K	450.29	Joback Method
cpg	296.48	J/mol×K	480.49	Joback Method
cpg	308.95	J/mol×K	510.69	Joback Method
cpg	320.84	J/mol×K	540.89	Joback Method
cpg	332.18	J/mol×K	571.09	Joback Method
cpg	342.98	J/mol×K	601.29	Joback Method
cpg	353.26	J/mol×K	631.49	Joback Method
dvisc	0.0054579	Pa×s	246.57	Joback Method

dvisc	0.0024654	Pa×s	280.52	Joback Method
dvisc	0.0013221	Pa×s	314.48	Joback Method
dvisc	0.0008006	Pa×s	348.43	Joback Method
dvisc	0.0005299	Pa×s	382.38	Joback Method
dvisc	0.0003752	Pa×s	416.34	Joback Method
dvisc	0.0002798	Pa×s	450.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368759&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