Heptan-2-yl formate

Inchi: InChI=1S/C8H16O2/c1-3-4-5-6-8(2)10-7-9/h7-8H,3-6H2,1-2H3
InchiKey: SEIYVCWCDDKKIS-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCCCCC(C)OC=O
Mol. weight [g/mol]: 144.21
CAS: 103884-53-3

Physical Properties

Property code	Value	Unit	Source
gf	-190.48	kJ/mol	Joback Method
hf	-431.53	kJ/mol	Joback Method
hfus	16.43	kJ/mol	Joback Method
hvap	42.14	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.128		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	969.40		NIST Webbook
tb	453.08	K	Joback Method
tc	627.37	K	Joback Method
tf	229.15	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.99	J/mol×K	453.08	Joback Method
cpg	293.22	J/mol×K	482.13	Joback Method
cpg	305.02	J/mol×K	511.18	Joback Method
cpg	316.38	J/mol×K	540.23	Joback Method
cpg	327.32	J/mol×K	569.27	Joback Method
cpg	337.83	J/mol×K	598.32	Joback Method
cpg	347.93	J/mol×K	627.37	Joback Method
dvisc	0.0055375	Pa×s	229.15	Joback Method

dvisc	0.0023301	Pa×s	266.47	Joback Method
dvisc	0.0012128	Pa×s	303.79	Joback Method
dvisc	0.0007283	Pa×s	341.12	Joback Method
dvisc	0.0004836	Pa×s	378.44	Joback Method
dvisc	0.0003456	Pa×s	415.76	Joback Method
dvisc	0.0002610	Pa×s	453.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103884533&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

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

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