

2-Pentanol, formate

Other names:	2-Pentyl formate
Inchi:	InChI=1S/C6H12O2/c1-3-4-6(2)8-5-7/h5-6H,3-4H2,1-2H3
InchiKey:	JNRQSKFTIYCDIP-UHFFFAOYSA-N
Formula:	C6H12O2
SMILES:	CCCC(C)OC=O
Mol. weight [g/mol]:	116.16
CAS:	58368-66-4

Physical Properties

Property code	Value	Unit	Source
gf	-207.32	kJ/mol	Joback Method
hf	-390.25	kJ/mol	Joback Method
hfus	11.25	kJ/mol	Joback Method
hvap	37.69	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.348		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	731.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	731.00		NIST Webbook
tb	407.32	K	Joback Method
tc	583.97	K	Joback Method
tf	206.61	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.69	J/molxK	407.32	Joback Method
cpg	211.53	J/molxK	436.76	Joback Method
cpg	221.04	J/molxK	466.20	Joback Method
cpg	230.24	J/molxK	495.64	Joback Method
cpg	239.12	J/molxK	525.08	Joback Method

cpg	247.68	J/mol×K	554.53	Joback Method
cpg	255.92	J/mol×K	583.97	Joback Method
dvisc	0.0052383	Paxs	206.61	Joback Method
dvisc	0.0022883	Paxs	240.06	Joback Method
dvisc	0.0012241	Paxs	273.51	Joback Method
dvisc	0.0007505	Paxs	306.97	Joback Method
dvisc	0.0005066	Paxs	340.42	Joback Method
dvisc	0.0003668	Paxs	373.87	Joback Method
dvisc	0.0002801	Paxs	407.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58368664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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