

Formic acid, 3,3-dimethylbut-2-yl ester

Inchi:	InChI=1S/C7H14O2/c1-6(9-5-8)7(2,3)4/h5-6H,1-4H3
InchiKey:	NQDIBLMCETWWEX-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	CC(OC=O)C(C)(C)C
Mol. weight [g/mol]:	130.18

Physical Properties

Property code	Value	Unit	Source
gf	-196.06	kJ/mol	Joback Method
hf	-419.64	kJ/mol	Joback Method
hfus	6.43	kJ/mol	Joback Method
hvap	38.62	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.594		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	818.00		NIST Webbook
tb	426.97	K	Joback Method
tc	613.91	K	Joback Method
tf	220.30	K	Joback Method
vc	0.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.49	J/mol×K	426.97	Joback Method
cpg	254.84	J/mol×K	458.13	Joback Method
cpg	266.61	J/mol×K	489.28	Joback Method
cpg	277.83	J/mol×K	520.44	Joback Method
cpg	288.51	J/mol×K	551.60	Joback Method
cpg	298.66	J/mol×K	582.75	Joback Method
cpg	308.31	J/mol×K	613.91	Joback Method
dvisc	0.0089081	Paxs	220.30	Joback Method
dvisc	0.0034139	Paxs	254.75	Joback Method

dvisc	0.0016442	Paxs	289.19	Joback Method
dvisc	0.0009251	Paxs	323.63	Joback Method
dvisc	0.0005814	Paxs	358.08	Joback Method
dvisc	0.0003964	Paxs	392.52	Joback Method
dvisc	0.0002875	Paxs	426.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U368205&Units=SI

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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