

Formic acid, 2,3-dimethylphenyl ester

Inchi:	InChI=1S/C9H10O2/c1-7-4-3-5-9(8(7)2)11-6-10/h3-6H,1-2H3
InchiKey:	ZHCRALNPDAMNAX-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	Cc1cccc(OC=O)c1C
Mol. weight [g/mol]:	150.17

Physical Properties

Property code	Value	Unit	Source
gf	-86.47	kJ/mol	Joback Method
hf	-233.30	kJ/mol	Joback Method
hfus	15.81	kJ/mol	Joback Method
hvap	48.36	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.839		Crippen Method
mvol	121.350	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	1207.00		NIST Webbook
tb	513.04	K	Joback Method
tc	726.15	K	Joback Method
tf	306.88	K	Joback Method
vc	0.467	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.40	J/molxK	513.04	Joback Method
cpg	268.93	J/molxK	548.56	Joback Method
cpg	279.91	J/molxK	584.08	Joback Method
cpg	290.33	J/molxK	619.60	Joback Method
cpg	300.20	J/molxK	655.12	Joback Method
cpg	309.53	J/molxK	690.64	Joback Method
cpg	318.32	J/molxK	726.15	Joback Method
dvisc	0.0014682	Paxs	306.88	Joback Method
dvisc	0.0009264	Paxs	341.24	Joback Method

dvisc	0.0006359	Paxs	375.60	Joback Method
dvisc	0.0004649	Paxs	409.96	Joback Method
dvisc	0.0003568	Paxs	444.32	Joback Method
dvisc	0.0002844	Paxs	478.68	Joback Method
dvisc	0.0002337	Paxs	513.04	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=U368917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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