

Formic acid, (3-methylphenyl)methyl ester

Inchi:	InChI=1S/C9H10O2/c1-8-3-2-4-9(5-8)6-11-7-10/h2-5,7H,6H2,1H3
InchiKey:	RWRCJBIEGCHXGW-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	Cc1cccc(COC=O)c1
Mol. weight [g/mol]:	150.17

Physical Properties

Property code	Value	Unit	Source
gf	-76.84	kJ/mol	Joback Method
hf	-221.83	kJ/mol	Joback Method
hfus	16.20	kJ/mol	Joback Method
hvap	47.70	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.668		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1193.00		NIST Webbook
tb	508.06	K	Joback Method
tc	719.99	K	Joback Method
tf	294.36	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.62	J/molxK	508.06	Joback Method
cpg	310.99	J/molxK	684.67	Joback Method
cpg	301.51	J/molxK	649.35	Joback Method
cpg	291.44	J/molxK	614.02	Joback Method
cpg	280.78	J/molxK	578.70	Joback Method
cpg	269.51	J/molxK	543.38	Joback Method
cpg	319.90	J/molxK	719.99	Joback Method
dvisc	0.0002417	Paxs	508.06	Joback Method
dvisc	0.0002999	Paxs	472.44	Joback Method

dvisc	0.0003855	Paxs	436.83	Joback Method
dvisc	0.0005181	Paxs	401.21	Joback Method
dvisc	0.0007377	Paxs	365.59	Joback Method
dvisc	0.0011334	Paxs	329.98	Joback Method
dvisc	0.0019322	Paxs	294.36	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=U368972&Units=SI

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_cvol:	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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