

Formic acid, 2-(4-chlorophenyl)ethyl ester

Inchi:	InChI=1S/C9H9ClO2/c10-9-3-1-8(2-4-9)5-6-12-7-11/h1-4,7H,5-6H2
InchiKey:	GQUHLGKYJKTSGT-UHFFFAOYSA-N
Formula:	C9H9ClO2
SMILES:	O=COCCc1ccc(Cl)cc1
Mol. weight [g/mol]:	184.62

Physical Properties

Property code	Value	Unit	Source
gf	-88.77	kJ/mol	Joback Method
hf	-237.57	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.055		Crippen Method
mvol	133.590	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinpol	1398.00		NIST Webbook
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tb	545.49	K	Joback Method
tc	762.26	K	Joback Method
tf	324.28	K	Joback Method
vc	0.515	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.18	J/molxK	545.49	Joback Method
cpg	293.39	J/molxK	581.62	Joback Method
cpg	303.95	J/molxK	617.75	Joback Method
cpg	313.88	J/molxK	653.88	Joback Method
cpg	323.19	J/molxK	690.01	Joback Method
cpg	331.89	J/molxK	726.13	Joback Method
cpg	340.01	J/molxK	762.26	Joback Method
dvisc	0.0019031	Paxs	324.28	Joback Method

dvisc	0.0011406	Paxs	361.15	Joback Method
dvisc	0.0007517	Paxs	398.02	Joback Method
dvisc	0.0005316	Paxs	434.88	Joback Method
dvisc	0.0003969	Paxs	471.75	Joback Method
dvisc	0.0003092	Paxs	508.62	Joback Method
dvisc	0.0002491	Paxs	545.49	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=U367881&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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