

Acetic acid, (4-chloro-2-methoxyphenyl)methyl ester

Inchi:	InChI=1S/C10H11ClO3/c1-7(12)14-6-8-3-4-9(11)5-10(8)13-2/h3-5H,6H2,1-2H3
InchiKey:	VOCDVPFIXYYVMF-UHFFFAOYSA-N
Formula:	C10H11ClO3
SMILES:	<chem>COc1cc(Cl)ccc1COC(C)=O</chem>
Mol. weight [g/mol]:	214.65

Physical Properties

Property code	Value	Unit	Source
gf	-224.38	kJ/mol	Joback Method
hf	-428.90	kJ/mol	Joback Method
hfus	23.09	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.412		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1589.00		NIST Webbook
rinpol	1589.00		NIST Webbook
tb	600.98	K	Joback Method
tc	817.52	K	Joback Method
tf	378.23	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.51	J/molxK	600.98	Joback Method
cpg	402.34	J/molxK	781.43	Joback Method
cpg	392.89	J/molxK	745.34	Joback Method
cpg	382.77	J/molxK	709.25	Joback Method
cpg	372.00	J/molxK	673.16	Joback Method
cpg	360.58	J/molxK	637.07	Joback Method
cpg	411.11	J/molxK	817.52	Joback Method
dvisc	0.0001655	Paxs	600.98	Joback Method

dvisc	0.0002025	Paxs	563.86	Joback Method
dvisc	0.0002551	Paxs	526.73	Joback Method
dvisc	0.0003327	Paxs	489.61	Joback Method
dvisc	0.0004531	Paxs	452.48	Joback Method
dvisc	0.0006524	Paxs	415.36	Joback Method
dvisc	0.0010088	Paxs	378.23	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=U368242&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
logp:	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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