

Phenylacetic acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C14H11ClO2/c15-12-6-8-13(9-7-12)17-14(16)10-11-4-2-1-3-5-11/h1-9H,10H2
InchiKey:	WQHZGESHVIOHHW-UHFFFAOYSA-N
Formula:	C14H11ClO2
SMILES:	O=C(Cc1ccccc1)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	246.69

Physical Properties

Property code	Value	Unit	Source
gf	36.34	kJ/mol	Joback Method
hf	-131.24	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	65.51	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.488		Crippen Method
mvol	180.280	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1873.00		NIST Webbook
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tb	691.78	K	Joback Method
tc	938.00	K	Joback Method
tf	414.98	K	Joback Method
vc	0.676	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.76	J/molxK	691.78	Joback Method
cpg	497.64	J/molxK	896.96	Joback Method
cpg	488.18	J/molxK	855.92	Joback Method
cpg	477.72	J/molxK	814.89	Joback Method
cpg	466.19	J/molxK	773.85	Joback Method
cpg	453.56	J/molxK	732.82	Joback Method
cpg	506.14	J/molxK	938.00	Joback Method
dvisc	0.0001408	Paxs	691.78	Joback Method

dvisc	0.0001765	Paxs	645.65	Joback Method
dvisc	0.0002289	Paxs	599.51	Joback Method
dvisc	0.0003102	Paxs	553.38	Joback Method
dvisc	0.0004441	Paxs	507.25	Joback Method
dvisc	0.0006831	Paxs	461.11	Joback Method
dvisc	0.0011566	Paxs	414.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307531&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
mccvol:	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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