

Phenylacetic acid, 4-chloro-, hexyl ester

Inchi:	InChI=1S/C14H19ClO2/c1-2-3-4-5-10-17-14(16)11-12-6-8-13(15)9-7-12/h6-9H,2-5,10-11
InchiKey:	ZRHSSOVTRTYRTE-UHFFFAOYSA-N
Formula:	C14H19ClO2
SMILES:	CCCCCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	254.75

Physical Properties

Property code	Value	Unit	Source
gf	-76.07	kJ/mol	Joback Method
hf	-367.77	kJ/mol	Joback Method
hfus	32.65	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.006		Crippen Method
mvol	204.040	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1840.00		NIST Webbook
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tb	665.10	K	Joback Method
tc	869.77	K	Joback Method
tf	388.56	K	Joback Method
vc	0.784	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.84	J/mol×K	665.10	Joback Method
cpg	537.98	J/mol×K	699.21	Joback Method
cpg	552.23	J/mol×K	733.32	Joback Method
cpg	565.61	J/mol×K	767.43	Joback Method
cpg	578.16	J/mol×K	801.55	Joback Method
cpg	589.90	J/mol×K	835.66	Joback Method
cpg	600.85	J/mol×K	869.77	Joback Method
dvisc	0.0013958	Paxs	388.56	Joback Method

dvisc	0.0007761	Paxs	434.65	Joback Method
dvisc	0.0004830	Paxs	480.74	Joback Method
dvisc	0.0003266	Paxs	526.83	Joback Method
dvisc	0.0002352	Paxs	572.92	Joback Method
dvisc	0.0001778	Paxs	619.01	Joback Method
dvisc	0.0001398	Paxs	665.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406210&Units=SI
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

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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