Phenylacetic acid, 4-chloro-, octyl ester

Inchi: InChI=1S/C16H23ClO2/c1-2-3-4-5-6-7-12-19-16(18)13-14-8-10-15(17)11-9-14/h8-11H,2-
InchiKey: KXKWBFXGXVAMQO-UHFFFAOYSA-N
Formula: C16H23ClO2
SMILES: CCCCCCCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 282.81

Physical Properties

Property code	Value	Unit	Source
gf	-59.23	kJ/mol	Joback Method
hf	-409.05	kJ/mol	Joback Method
hfus	37.83	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.786		Crippen Method
mcvol	232.220	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	710.86	K	Joback Method
tc	910.76	K	Joback Method
tf	411.10	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.76	J/mol×K	710.86	Joback Method
cpg	645.71	J/mol×K	744.18	Joback Method
cpg	660.72	J/mol×K	777.49	Joback Method
cpg	674.83	J/mol×K	810.81	Joback Method
cpg	688.05	J/mol×K	844.12	Joback Method
cpg	700.42	J/mol×K	877.44	Joback Method
cpg	711.96	J/mol×K	910.76	Joback Method
dvisc	0.0012148	Pa×s	411.10	Joback Method

dvisc	0.0006558	Pa×s	461.06	Joback Method
dvisc	0.0003994	Pa×s	511.02	Joback Method
dvisc	0.0002657	Pa×s	560.98	Joback Method
dvisc	0.0001889	Pa×s	610.94	Joback Method
dvisc	0.0001415	Pa×s	660.90	Joback Method
dvisc	0.0001103	Pa×s	710.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U406212&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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