

Phenylacetic acid, 4-chloro-, nonyl ester

Inchi:	InChI=1S/C17H25ClO2/c1-2-3-4-5-6-7-8-13-20-17(19)14-15-9-11-16(18)12-10-15/h9-12H
InchiKey:	CIJNAOYNVHUVIP-UHFFFAOYSA-N
Formula:	C17H25ClO2
SMILES:	CCCCCCCCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	296.83

Physical Properties

Property code	Value	Unit	Source
gf	-50.81	kJ/mol	Joback Method
hf	-429.69	kJ/mol	Joback Method
hfus	40.42	kJ/mol	Joback Method
hvap	69.92	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.176		Crippen Method
mvol	246.310	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2152.00		NIST Webbook
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tb	733.74	K	Joback Method
tc	931.90	K	Joback Method
tf	422.37	K	Joback Method
vc	0.953	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.02	J/molxK	733.74	Joback Method
cpg	701.30	J/molxK	766.77	Joback Method
cpg	716.62	J/molxK	799.79	Joback Method
cpg	731.01	J/molxK	832.82	Joback Method
cpg	744.50	J/molxK	865.85	Joback Method
cpg	757.11	J/molxK	898.87	Joback Method
cpg	768.87	J/molxK	931.90	Joback Method
dvisc	0.0011220	Paxs	422.37	Joback Method

dvisc	0.0005974	Paxs	474.26	Joback Method
dvisc	0.0003602	Paxs	526.16	Joback Method
dvisc	0.0002378	Paxs	578.06	Joback Method
dvisc	0.0001681	Paxs	629.95	Joback Method
dvisc	0.0001253	Paxs	681.85	Joback Method
dvisc	0.0000974	Paxs	733.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406213&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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