

Phenylacetic acid, 4-chloro-, butyl ester

Inchi:	InChI=1S/C12H15ClO2/c1-2-3-8-15-12(14)9-10-4-6-11(13)7-5-10/h4-7H,2-3,8-9H2,1H3
InchiKey:	RYVAYVLGDLRUIN-UHFFFAOYSA-N
Formula:	C12H15ClO2
SMILES:	CCCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	226.70

Physical Properties

Property code	Value	Unit	Source
gf	-92.91	kJ/mol	Joback Method
hf	-326.49	kJ/mol	Joback Method
hfus	27.47	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.226		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1642.00		NIST Webbook
tb	619.34	K	Joback Method
tc	830.22	K	Joback Method
tf	366.02	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.33	J/molxK	619.34	Joback Method
cpg	435.34	J/molxK	654.49	Joback Method
cpg	448.54	J/molxK	689.63	Joback Method
cpg	460.94	J/molxK	724.78	Joback Method
cpg	472.56	J/molxK	759.93	Joback Method
cpg	483.41	J/molxK	795.07	Joback Method
cpg	493.53	J/molxK	830.22	Joback Method
dvisc	0.0015544	Paxs	366.02	Joback Method
dvisc	0.0008929	Paxs	408.24	Joback Method

dvisc	0.0005690	Paxs	450.46	Joback Method
dvisc	0.0003918	Paxs	492.68	Joback Method
dvisc	0.0002861	Paxs	534.90	Joback Method
dvisc	0.0002188	Paxs	577.12	Joback Method
dvisc	0.0001735	Paxs	619.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406208&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

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

Latest version available from:

<https://www.chemeo.com/cid/91-274-7/Phenylacetic-acid-4-chloro-butyl-ester.pdf>

Generated by Cheméo on 2024-04-26 13:46:01.168269497 +0000 UTC m=+16428410.088846819.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.