3-Phenoxybenzyl chloride

Inchi: InChI=1S/C13H11ClO/c14-10-11-5-4-8-13(9-11)15-12-6-2-1-3-7-12/h1-9H,10H2
InchiKey: QUYVTGFWFHQVRO-UHFFFAOYSA-N
Formula: C13H11ClO
SMILES: ClCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 218.68

Physical Properties

Property code	Value	Unit	Source
gf	156.84	kJ/mol	Joback Method
hf	1.98	kJ/mol	Joback Method
hfus	22.50	kJ/mol	Joback Method
hvap	56.54	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	4.218		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1773.00		NIST Webbook
tb	615.03	K	Joback Method
tc	860.59	K	Joback Method
tf	353.78	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.84	J/mol×K	615.03	Joback Method
cpg	390.88	J/mol×K	655.96	Joback Method
cpg	404.77	J/mol×K	696.88	Joback Method
cpg	417.56	J/mol×K	737.81	Joback Method
cpg	429.30	J/mol×K	778.74	Joback Method
cpg	440.03	J/mol×K	819.66	Joback Method
cpg	449.81	J/mol×K	860.59	Joback Method
dvisc	0.0013816	Pa×s	353.78	Joback Method
dvisc	0.0007805	Pa×s	397.32	Joback Method

dvisc	0.0004936	Pa×s	440.86	Joback Method
dvisc	0.0003390	Pa×s	484.40	Joback Method
dvisc	0.0002476	Pa×s	527.95	Joback Method
dvisc	0.0001898	Pa×s	571.49	Joback Method
dvisc	0.0001510	Pa×s	615.03	Joback Method

Sources

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=U353822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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