

2-(4-Chlorophenoxy)tetrahydro-2h-pyran

Inchi:	InChI=1S/C11H13ClO2/c12-9-4-6-10(7-5-9)14-11-3-1-2-8-13-11/h4-7,11H,1-3,8H2
InchiKey:	BATPOJJUDDURGW-UHFFFAOYSA-N
Formula:	C11H13ClO2
SMILES:	Clc1ccc(OC2CCCCO2)cc1
Mol. weight [g/mol]:	212.67
CAS:	20443-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-34.08	kJ/mol	Joback Method
hf	-270.95	kJ/mol	Joback Method
hfus	23.10	kJ/mol	Joback Method
hvap	54.75	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.245		Crippen Method
mcvol	155.210	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	589.09	K	Joback Method
tc	833.56	K	Joback Method
tf	338.77	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.24	J/molxK	589.09	Joback Method
cpg	390.72	J/molxK	629.84	Joback Method
cpg	406.97	J/molxK	670.58	Joback Method
cpg	422.01	J/molxK	711.33	Joback Method
cpg	435.87	J/molxK	752.07	Joback Method
cpg	448.58	J/molxK	792.82	Joback Method
cpg	460.18	J/molxK	833.56	Joback Method
dvisc	0.0022508	Paxs	338.77	Joback Method
dvisc	0.0011885	Paxs	380.49	Joback Method

dvisc	0.0007120	Paxs	422.21	Joback Method
dvisc	0.0004677	Paxs	463.93	Joback Method
dvisc	0.0003293	Paxs	505.65	Joback Method
dvisc	0.0002446	Paxs	547.37	Joback Method
dvisc	0.0001895	Paxs	589.09	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=C20443907&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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