Dichlorphen, O,O'-(4-chlorobutyryl)-

Other names: Dichlorphen, O,O'-(4-chlorobutyl)-
Inchi: InChI=1S/C21H20Cl4O4/c22-9-1-3-20(26)28-18-7-5-16(24)12-14(18)11-15-13-17(25)6-8
InchiKey: MCVRVTRTTXRFTM-UHFFFAOYSA-N
Formula: C21H20Cl4O4
SMILES: O=C(CCCCl)Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)CCCCl
Mol. weight [g/mol]: 478.19

Physical Properties

Property code	Value	Unit	Source
gf	-203.32	kJ/mol	Joback Method
hf	-602.15	kJ/mol	Joback Method
hfus	59.03	kJ/mol	Joback Method
hvap	105.39	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	6.433		Crippen Method
mcvol	323.070	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	3291.00		NIST Webbook
rinpol	3291.00		NIST Webbook
tb	1055.46	K	Joback Method
tc	1298.61	K	Joback Method
tf	693.35	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.45	J/mol×K	1055.46	Joback Method
cpg	944.50	J/mol×K	1258.09	Joback Method
cpg	941.23	J/mol×K	1217.56	Joback Method
cpg	936.74	J/mol×K	1177.04	Joback Method
cpg	930.97	J/mol×K	1136.51	Joback Method
cpg	923.88	J/mol×K	1095.99	Joback Method
cpg	946.57	J/mol×K	1298.61	Joback Method

dvisc	0.0000273	Pa×s	1055.46	Joback Method
dvisc	0.0000335	Pa×s	995.11	Joback Method
dvisc	0.0000422	Pa×s	934.76	Joback Method
dvisc	0.0000550	Pa×s	874.40	Joback Method
dvisc	0.0000744	Pa×s	814.05	Joback Method
dvisc	0.0001057	Pa×s	753.70	Joback Method
dvisc	0.0001597	Pa×s	693.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360648&Units=SI
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

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