Dichlorophen, O-(6-bromohexanoyl)-

Inchi: InChI=1S/C19H19BrCl2O3/c20-9-3-1-2-4-19(24)25-18-8-6-16(22)12-14(18)10-13-11-15(
InchiKey: DIHIWNGGTNTBLI-UHFFFAOYSA-N
Formula: C19H19BrCl2O3
SMILES: O=C(CCCCCBr)Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1O
Mol. weight [g/mol]: 446.16

Physical Properties

Property code	Value	Unit	Source
gf	-93.05	kJ/mol	Joback Method
hf	-424.10	kJ/mol	Joback Method
hfus	54.13	kJ/mol	Joback Method
hvap	101.80	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.151		Crippen Method
mcvol	286.340	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	3557.00		NIST Webbook
rinpol	3557.00		NIST Webbook
tb	1000.35	K	Joback Method
tc	1247.06	K	Joback Method
tf	697.81	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.04	J/mol×K	1000.35	Joback Method
cpg	821.33	J/mol×K	1041.47	Joback Method
cpg	833.17	J/mol×K	1082.59	Joback Method
cpg	844.68	J/mol×K	1123.71	Joback Method
cpg	856.01	J/mol×K	1164.82	Joback Method
cpg	867.28	J/mol×K	1205.94	Joback Method
cpg	878.61	J/mol×K	1247.06	Joback Method
dvisc	0.0000196	Pa×s	697.81	Joback Method

dvisc	0.0000115	Pa×s	748.23	Joback Method
dvisc	0.0000072	Pa×s	798.66	Joback Method
dvisc	0.0000048	Pa×s	849.08	Joback Method
dvisc	0.0000033	Pa×s	899.50	Joback Method
dvisc	0.0000024	Pa×s	949.93	Joback Method
dvisc	0.0000018	Pa×s	1000.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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