Pretilachlor

Inchi: InChI=1S/C17H26ClNO2/c1-4-11-21-12-10-19(16(20)13-18)17-14(5-2)8-7-9-15(17)6-3/h
InchiKey: YLPGTOIOYRQOHV-UHFFFAOYSA-N
Formula: C17H26ClNO2
SMILES: CCCOCCN(C(=O)CCl)c1c(CC)cccc1CC
Mol. weight [g/mol]: 311.85
CAS: 81690-06-4

Physical Properties

Property code	Value	Unit	Source
gf	50.34	kJ/mol	Joback Method
hf	-373.63	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	72.62	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.810		Crippen Method
mcvol	256.290	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	2165.00		NIST Webbook
rinpol	2173.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2165.00		NIST Webbook
tb	751.16	K	Joback Method
tc	948.70	K	Joback Method
tf	467.36	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.34	J/mol×K	751.16	Joback Method
cpg	741.61	J/mol×K	784.08	Joback Method
cpg	756.90	J/mol×K	817.01	Joback Method
cpg	771.25	J/mol×K	849.93	Joback Method
cpg	784.69	J/mol×K	882.85	Joback Method

cpg	797.24	J/mol×K	915.78	Joback Method
cpg	808.95	J/mol×K	948.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81690064&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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