

Chlomethoxyfen

Other names:	X-52 2,4-Dichlorophenyl 3-methoxy-4-nitrophenyl ether
Inchi:	InChI=1S/C13H9Cl2NO4/c1-19-13-7-9(3-4-11(13)16(17)18)20-12-5-2-8(14)6-10(12)15/h
InchiKey:	DXXVCXKMSWHGTF-UHFFFAOYSA-N
Formula:	C13H9Cl2NO4
SMILES:	COc1cc(Oc2ccc(Cl)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	314.12
CAS:	32861-85-1

Physical Properties

Property code	Value	Unit	Source
gf	46.57	kJ/mol	Joback Method
hf	-191.15	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	81.91	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.703		Crippen Method
mcvol	200.150	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	2432.00		NIST Webbook
rinpol	2465.00		NIST Webbook
rinpol	2432.00		NIST Webbook
rinpol	2432.00		NIST Webbook
rinpol	2465.00		NIST Webbook
rinpol	2435.00		NIST Webbook
tb	841.66	K	Joback Method
tc	1105.22	K	Joback Method
tf	587.10	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.19	J/molxK	841.66	Joback Method

cpg	519.47	J/mol×K	885.59	Joback Method
cpg	528.53	J/mol×K	929.51	Joback Method
cpg	536.39	J/mol×K	973.44	Joback Method
cpg	543.07	J/mol×K	1017.36	Joback Method
cpg	548.57	J/mol×K	1061.29	Joback Method
cpg	552.91	J/mol×K	1105.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32861851&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
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

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