Fenoxanil, N-methyl-

Inchi: InChI=1S/C16H20Cl2N2O2/c1-10(2)16(4,9-19)20(5)15(21)11(3)22-14-7-6-12(17)8-13(14
InchiKey: ZFHSGHLOKSXRIQ-UHFFFAOYSA-N
Formula: C16H20Cl2N2O2
SMILES: CC(Oc1ccc(Cl)cc1Cl)C(=O)N(C)C(C)(C#N)C(C)C
Mol. weight [g/mol]: 343.25

Physical Properties

Property code	Value	Unit	Source
gf	161.13	kJ/mol	Joback Method
hf	-223.16	kJ/mol	Joback Method
hfus	31.71	kJ/mol	Joback Method
hvap	83.18	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.157		Crippen Method
mcvol	255.820	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	2327.00		NIST Webbook
tb	863.68	K	Joback Method
tc	1092.80	K	Joback Method
tf	523.42	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.63	J/mol×K	863.68	Joback Method
cpg	733.98	J/mol×K	901.87	Joback Method
cpg	745.33	J/mol×K	940.05	Joback Method
cpg	755.74	J/mol×K	978.24	Joback Method
cpg	765.30	J/mol×K	1016.43	Joback Method
cpg	774.06	J/mol×K	1054.62	Joback Method
cpg	782.11	J/mol×K	1092.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374836&Units=SI

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