Fenoxanil, N-pentafluoropropionyl-

Inchi: InChI=1S/C18H17Cl2F5N2O3/c1-9(2)16(4,8-26)27(15(29)17(21,22)18(23,24)25)14(28)1
InchiKey: ZIOIJIWERZSHCB-UHFFFAOYSA-N
Formula: C18H17Cl2F5N2O3
SMILES: CC(Oc1ccc(Cl)cc1Cl)C(=O)N(C(=O)C(F)(F)C(F)(F)F)C(C)(C#N)C(C)C
Mol. weight [g/mol]: 475.24

Physical Properties

Property code	Value	Unit	Source
gf	-919.32	kJ/mol	Joback Method
hf	-1375.07	kJ/mol	Joback Method
hfus	39.06	kJ/mol	Joback Method
hvap	87.71	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.252		Crippen Method
mcvol	294.420	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
tb	953.20	K	Joback Method
tc	1174.01	K	Joback Method
tf	603.68	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.54	J/mol×K	953.20	Joback Method
cpg	889.26	J/mol×K	990.00	Joback Method
cpg	898.30	J/mol×K	1026.80	Joback Method
cpg	906.79	J/mol×K	1063.60	Joback Method
cpg	914.84	J/mol×K	1100.40	Joback Method
cpg	922.57	J/mol×K	1137.21	Joback Method
cpg	930.10	J/mol×K	1174.01	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=U374338&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