Fenoxanil, N-trifluoroacetyl-

Inchi: InChI=1S/C17H17Cl2F3N2O3/c1-9(2)16(4,8-23)24(15(26)17(20,21)22)14(25)10(3)27-13
InchiKey: WUHAEAWFJHJBSI-UHFFFAOYSA-N
Formula: C17H17Cl2F3N2O3
SMILES: CC(Oc1ccc(Cl)cc1Cl)C(=O)N(C(=O)C(F)(F)F)C(C)(C#N)C(C)C
Mol. weight [g/mol]: 425.23

Physical Properties

Property code	Value	Unit	Source
gf	-540.96	kJ/mol	Joback Method
hf	-953.46	kJ/mol	Joback Method
hfus	37.72	kJ/mol	Joback Method
hvap	88.41	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.616		Crippen Method
mcvol	276.790	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2059.00		NIST Webbook
tb	935.01	K	Joback Method
tc	1158.56	K	Joback Method
tf	588.81	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.91	J/mol×K	935.01	Joback Method
cpg	817.77	J/mol×K	972.27	Joback Method
cpg	826.82	J/mol×K	1009.53	Joback Method
cpg	835.17	J/mol×K	1046.79	Joback Method
cpg	842.91	J/mol×K	1084.04	Joback Method
cpg	850.13	J/mol×K	1121.30	Joback Method
cpg	856.92	J/mol×K	1158.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374337&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