propoxur, TFA

Inchi: InChI=1S/C13H14F3NO4/c1-8(2)20-9-6-4-5-7-10(9)21-12(19)17(3)11(18)13(14,15)16/h4
InchiKey: XREPZIXVQDRNMM-UHFFFAOYSA-N
Formula: C13H14F3NO4
SMILES: CC(C)Oc1ccccc1OC(=O)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 305.25

Physical Properties

Property code	Value	Unit	Source
gf	-779.73	kJ/mol	Joback Method
hf	-1111.02	kJ/mol	Joback Method
hfus	29.98	kJ/mol	Joback Method
hvap	63.69	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.993		Crippen Method
mcvol	200.440	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1546.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1558.00		NIST Webbook
tb	687.66	K	Joback Method
tc	883.39	K	Joback Method
tf	441.19	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.40	J/mol×K	687.66	Joback Method
cpg	566.43	J/mol×K	720.28	Joback Method
cpg	578.58	J/mol×K	752.90	Joback Method
cpg	589.86	J/mol×K	785.53	Joback Method
cpg	600.31	J/mol×K	818.15	Joback Method
cpg	609.96	J/mol×K	850.77	Joback Method
cpg	618.85	J/mol×K	883.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522175&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