2,4,5-T, PFB

Other names: 2,4,5-T, PFB ester
Inchi: InChI=1S/C15H6Cl3F5O3/c16-6-1-8(18)9(2-7(6)17)25-4-10(24)26-3-5-11(19)13(21)15(23
InchiKey: AZTNACJVFYOPLN-UHFFFAOYSA-N
Formula: C15H6Cl3F5O3
SMILES: O=C(COc1cc(Cl)c(Cl)cc1Cl)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 435.56

Physical Properties

Property code	Value	Unit	Source
gf	-1125.56	kJ/mol	Joback Method
hf	-1376.42	kJ/mol	Joback Method
hfus	51.54	kJ/mol	Joback Method
hvap	79.47	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	5.465		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	2228.00		NIST Webbook
rinpol	2221.00		NIST Webbook
rinpol	2222.00		NIST Webbook
ripol	3366.00		NIST Webbook
ripol	3366.00		NIST Webbook
ripol	3336.00		NIST Webbook
tb	843.15	K	Joback Method
tc	1052.95	K	Joback Method
tf	598.91	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.74	J/mol×K	843.15	Joback Method
cpg	595.17	J/mol×K	878.12	Joback Method
cpg	602.77	J/mol×K	913.08	Joback Method

cpg	609.53	J/mol×K	948.05	Joback Method
cpg	615.44	J/mol×K	983.01	Joback Method
cpg	620.49	J/mol×K	1017.98	Joback Method
cpg	624.67	J/mol×K	1052.95	Joback Method

Sources

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=R13937&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume