2,4-DP, PFB ester

Other names: Dichlorprop, PFB
Dichlorprop, PFB ester
Inchi: InChI=1S/C16H9Cl2F5O3/c1-6(26-10-3-2-7(17)4-9(10)18)16(24)25-5-8-11(19)13(21)15(
InchiKey: PCROGCAYPVHGSU-UHFFFAOYSA-N
Formula: C16H9Cl2F5O3
SMILES: CC(Oc1ccc(Cl)cc1Cl)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 415.14

Physical Properties

Property code	Value	Unit	Source
gf	-1098.02	kJ/mol	Joback Method
hf	-1375.13	kJ/mol	Joback Method
hfus	46.80	kJ/mol	Joback Method
hvap	76.26	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.200		Crippen Method
mcvol	235.420	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2043.00		NIST Webbook
rinpol	2038.00		NIST Webbook
rinpol	2035.00		NIST Webbook
ripol	2757.00		NIST Webbook
ripol	2758.00		NIST Webbook
ripol	2790.00		NIST Webbook
ripol	2757.00		NIST Webbook
tb	823.18	K	Joback Method
tc	1029.67	K	Joback Method
tf	552.74	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.83	J/mol×K	823.18	Joback Method

cpg	632.84	J/mol×K	857.59	Joback Method
cpg	641.97	J/mol×K	892.01	Joback Method
cpg	650.22	J/mol×K	926.42	Joback Method
cpg	657.59	J/mol×K	960.84	Joback Method
cpg	664.08	J/mol×K	995.25	Joback Method
cpg	669.67	J/mol×K	1029.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R13973&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume