(2,4-Dichlorophenoxy)acetic acid, pentafluorobenzyl ester

Other names: 2,4-Dichlorophenoxyacetic acid, pentafluorophenylmethyl ester
2,4-D, PFB
2,4-D PFB ester

Inchi: InChI=1S/C15H7Cl2F5O3/c16-6-1-2-9(8(17)3-6)24-5-10(23)25-4-7-11(18)13(20)15(22)14

InchiKey: PZSLTUFVPUDAQF-UHFFFAOYSA-N

Formula: C15H7Cl2F5O3

SMILES: O=C(COc1ccc(Cl)cc1Cl)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 401.11

CAS: 68704-50-7

Physical Properties

Property code	Value	Unit	Source
gf	-1104.00	kJ/mol	Joback Method
hf	-1349.21	kJ/mol	Joback Method
hfus	47.73	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	4.811		Crippen Method
mcvol	221.330	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	2081.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2081.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2089.00		NIST Webbook
ripol	2980.00		NIST Webbook
ripol	3021.00		NIST Webbook
ripol	2980.00		NIST Webbook
tb	800.74	K	Joback Method
tc	1005.61	K	Joback Method
tf	556.47	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.69	J/mol×K	800.74	Joback Method
cpg	578.18	J/mol×K	834.89	Joback Method
cpg	586.88	J/mol×K	869.03	Joback Method
cpg	594.77	J/mol×K	903.18	Joback Method
cpg	601.87	J/mol×K	937.32	Joback Method
cpg	608.15	J/mol×K	971.47	Joback Method
cpg	613.61	J/mol×K	1005.61	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=C68704507&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume