3,6-Dichloro-2-methoxybenzoic acid,pentafluorobenzyl ester

Other names: Dicamba, PFB

Dicamba, PFB ester

Inchi: InChI=1S/C15H7Cl2F5O3/c1-24-14-7(17)3-2-6(16)8(14)15(23)25-4-5-9(18)11(20)13(22)

InchiKey: GJDVJKOVZTUAOF-UHFFFAOYSA-N

Formula: C15H7Cl2F5O3

SMILES: COc1c(Cl)ccc(Cl)c1C(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 401.11

CAS: 84949-26-8

Physical Properties

Property code	Value	Unit	Source
gf	-1113.63	kJ/mol	Joback Method
hf	-1360.68	kJ/mol	Joback Method
hfus	47.34	kJ/mol	Joback Method
hvap	75.08	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	5.055		Crippen Method
mcvol	221.330	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
tb	805.72	K	Joback Method
tc	1011.40	K	Joback Method
tf	568.99	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.00	J/mol×K	805.72	Joback Method
cpg	576.41	J/mol×K	840.00	Joback Method
cpg	585.04	J/mol×K	874.28	Joback Method
cpg	592.87	J/mol×K	908.56	Joback Method
cpg	599.88	J/mol×K	942.84	Joback Method
cpg	606.07	J/mol×K	977.12	Joback Method
cpg	611.41	J/mol×K	1011.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84949268&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume