

MCPP PFB ester

Other names:	Mecoprop, PFB ester Mecoprop, PFB
Inchi:	InChI=1S/C17H12ClF5O3/c1-7-5-9(18)3-4-11(7)26-8(2)17(24)25-6-10-12(19)14(21)16(2)
InchiKey:	SJFSFUDCTAJWJN-UHFFFAOYSA-N
Formula:	C17H12ClF5O3
SMILES:	<chem>Cc1cc(Cl)ccc1OC(C)C(=O)OCc1c(F)c(F)c(F)c(F)c1F</chem>
Mol. weight [g/mol]:	394.72

Physical Properties

Property code	Value	Unit	Source
gf	-1077.67	kJ/mol	Joback Method
hf	-1380.03	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	74.10	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	4.855		Crippen Method
mcvol	237.270	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	1974.00		NIST Webbook
rinpol	1977.00		NIST Webbook
ripol	2620.00		NIST Webbook
ripol	2619.00		NIST Webbook
tb	808.63	K	Joback Method
tc	1010.29	K	Joback Method
tf	534.09	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.17	J/molxK	808.63	Joback Method
cpg	666.60	J/molxK	842.24	Joback Method
cpg	677.12	J/molxK	875.85	Joback Method
cpg	686.76	J/molxK	909.46	Joback Method

cpg	695.49	J/mol×K	943.07	Joback Method
cpg	703.32	J/mol×K	976.68	Joback Method
cpg	710.24	J/mol×K	1010.29	Joback Method

Sources

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=R14046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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