MCPB, PFB

Other names: MCPB, PFB ester
Inchi: InChI=1S/C18H14ClF5O3/c1-9-7-10(19)4-5-12(9)26-6-2-3-13(25)27-8-11-14(20)16(22)18
InchiKey: VLHQFFHQFQRFIP-UHFFFAOYSA-N
Formula: C18H14ClF5O3
SMILES: Cc1cc(Cl)ccc1OCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 408.75

Physical Properties

Property code	Value	Unit	Source
gf	-1066.81	kJ/mol	Joback Method
hf	-1395.39	kJ/mol	Joback Method
hfus	51.31	kJ/mol	Joback Method
hvap	76.71	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.246		Crippen Method
mcvol	251.360	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2257.00		NIST Webbook
ripol	3147.00		NIST Webbook
tb	831.95	K	Joback Method
tc	1031.66	K	Joback Method
tf	560.36	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.78	J/mol×K	831.95	Joback Method
cpg	721.45	J/mol×K	865.23	Joback Method
cpg	732.19	J/mol×K	898.52	Joback Method
cpg	742.02	J/mol×K	931.80	Joback Method
cpg	750.92	J/mol×K	965.09	Joback Method
cpg	758.91	J/mol×K	998.37	Joback Method
cpg	765.97	J/mol×K	1031.66	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=R13991&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