2,4,5-TB PFB ester

Inchi: InChI=1S/C17H10Cl3F5O3/c18-8-4-10(20)11(5-9(8)19)27-3-1-2-12(26)28-6-7-13(21)15(2
InchiKey: ABFWDLIGMFYBPC-UHFFFAOYSA-N
Formula: C17H10Cl3F5O3
SMILES: O=C(CCCOc1cc(Cl)c(Cl)cc1Cl)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 463.61

Physical Properties

Property code	Value	Unit	Source
gf	-1108.72	kJ/mol	Joback Method
hf	-1417.70	kJ/mol	Joback Method
hfus	56.72	kJ/mol	Joback Method
hvap	83.92	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	6.245		Crippen Method
mcvol	261.750	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2481.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	888.91	K	Joback Method
tc	1098.91	K	Joback Method
tf	621.45	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.42	J/mol×K	888.91	Joback Method
cpg	704.57	J/mol×K	923.91	Joback Method
cpg	712.77	J/mol×K	958.91	Joback Method
cpg	720.02	J/mol×K	993.91	Joback Method
cpg	726.31	J/mol×K	1028.91	Joback Method
cpg	731.63	J/mol×K	1063.91	Joback Method
cpg	735.99	J/mol×K	1098.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R14000&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume