CPIB PFB ester

Other names: Clofibric acid, PFB
Inchi: InChI=1S/C17H12ClF5O3/c1-17(2,26-9-5-3-8(18)4-6-9)16(24)25-7-10-11(19)13(21)15(23
InchiKey: LWCTUOXYEKQVKP-UHFFFAOYSA-N
Formula: C17H12ClF5O3
SMILES: CC(C)(Oc1ccc(Cl)cc1)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 394.72

Physical Properties

Property code	Value	Unit	Source
gf	-1062.76	kJ/mol	Joback Method
hf	-1372.03	kJ/mol	Joback Method
hfus	41.69	kJ/mol	Joback Method
hvap	72.53	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	4.936		Crippen Method
mcvol	237.270	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1934.00		NIST Webbook
ripol	2603.00		NIST Webbook
ripol	2525.00		NIST Webbook
ripol	2525.00		NIST Webbook
tb	800.86	K	Joback Method
tc	1005.98	K	Joback Method
tf	538.99	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.84	J/mol×K	800.86	Joback Method
cpg	669.29	J/mol×K	835.05	Joback Method
cpg	679.83	J/mol×K	869.23	Joback Method
cpg	689.50	J/mol×K	903.42	Joback Method

cpg	698.30	J/mol×K	937.61	Joback Method
cpg	706.25	J/mol×K	971.79	Joback Method
cpg	713.38	J/mol×K	1005.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R14032&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume