Fenofibrate

Other names:	2-(4-(4-Chlorobenzoyl)phenoxy)-2-methylpropanoic acid 1-methylethyl ester
	2-[4-(4-Chlorobenzoyl)phenoxy]-2-methylpropanoic acid, isopropyl ester
	(fenofibrate)
	Ankebin
	Antara
	Elasterin
	Fenobrate
	Fenogal
	Fenotard
	Isopropyl (4'-(p-chlorobenzoyl)-2-phenoxy-2-methyl)propionate
	Isopropyl 2-[p-(p-chlorobenzoyl)phenoxy]-2-methylpropionate
	Lipanthyl
	Lipantil
	Lipidex
	Lipidil
	Lipifen
	Lipirex
	Lipoclar
	Lipofene
	Liposit
	Lipsin
	NSC 281319
	Nolipax
	Procetofen
	Procetofene
	Procetoken
	Proctofene
	Propanoic acid, 2-[4-(4-chlorobenzoyl)phenoxy]-2-methyl-, 1-methylethyl ester
	Protolipan
	Secalip
	Sedufen
	Tricor
Inchi:	InChI=1S/C20H21ClO4/c1-13(2)24-19(23)20(3,4)25-17-11-7-15(8-12-17)18(22)14-5-9-16
InchiKey:	YMTINGFKWWXKFG-UHFFFAOYSA-N
Formula:	C20H21ClO4
SMILES:	CC(C)OC(=O)C(C)(C)Oc1ccc(C(=O)c2ccc(Cl)cc2)cc1
Mol. weight [g/mol]:	360.83
CAS:	49562-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-156.29	kJ/mol	Joback Method
hf	-525.38	kJ/mol	Joback Method
hfus	33.69	kJ/mol	Joback Method
hvap	87.00	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.680		Crippen Method
mcvol	272.260	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
tb	906.66	K	Joback Method
tc	1145.97	K	Joback Method
tf	353.62	K	Solubility of Fenofibrate in Different Binary Solvents: Experimental Data and Results of Thermodynamic Modeling
tf	355.15	K	Phase equilibria of the binary systems of fenofibrate and dense gases (carbon dioxide, propane, trifluoromethane)
tf	354.75	K	Differential scanning calorimetry and thermally stimulated depolarization currents study on the molecular dynamics in amorphous fenofibrate
tf	352.05	K	Thermodynamics of fenofibrate and solubility in pure organic solvents
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.77	J/mol×K	906.66	Joback Method
cpg	817.86	J/mol×K	946.54	Joback Method
cpg	829.62	J/mol×K	986.43	Joback Method
cpg	840.13	J/mol×K	1026.31	Joback Method
cpg	849.45	J/mol×K	1066.20	Joback Method
cpg	857.66	J/mol×K	1106.08	Joback Method
cpg	864.82	J/mol×K	1145.97	Joback Method

dvisc	0.0003631	Pa×s	554.70	Joback Method
dvisc	0.0002040	Pa×s	613.36	Joback Method
dvisc	0.0001268	Pa×s	672.02	Joback Method
dvisc	0.0000850	Pa×s	730.68	Joback Method
dvisc	0.0000605	Pa×s	789.34	Joback Method
dvisc	0.0000451	Pa×s	848.00	Joback Method
dvisc	0.0000350	Pa×s	906.66	Joback Method
hfust	32.40	kJ/mol	353.70	NIST Webbook

Sources

Thermodynamics of fenofibrate and solubility in pure organic solvents:	https://www.doi.org/10.1016/j.fluid.2014.01.029
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Differential scanning calorimetry and thermally stimulated depolarization currents study on the molecular dynamics of amorphous fenofibrate:	https://www.doi.org/10.1016/j.tca.2015.11.012
Solubility of Fenofibrate in Different Binary Solvents: Experimental Data and Results of Thermodynamic Modeling:	https://www.doi.org/10.1021/acs.jced.6b00268
McGowan's Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49562289&Units=SI
Phase equilibria of the binary systems of fenofibrate and dense gases (carbon dioxide, propane, trifluoromethane):	https://www.doi.org/10.1016/j.fluid.2018.07.018

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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