Gemfibrozil

Other names:	2,2-Dimethyl-5-(2,5-xylyloxy)valeric acid
	5-(2,5-Dimethylphenoxy)-2,2-dimethylpentanoic acid
	CI-719
	Lopid
	Pentanoic acid, 5-(2,5-dimethylphenoxy)-2,2-dimethyl-
	Valeric acid, 2,2-dimethyl-5-(2,5-xylyloxy)-
Inchi:	InChI=1S/C15H22O3/c1-11-6-7-12(2)13(10-11)18-9-5-8-15(3,4)14(16)17/h6-7,10H,5,8-9
InchiKey:	HEMJJKBWTPKOJG-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	Cc1ccc(C)c(OCCCC(C)(C)C(=O)O)c1
Mol. weight [g/mol]:	250.33
CAS:	25812-30-0

Physical Properties

Property code	Value	Unit	Source
gf	-199.33	kJ/mol	Joback Method
hf	-545.12	kJ/mol	Joback Method
hfus	27.33	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.573		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
tb	744.48	K	Joback Method
tc	943.39	K	Joback Method
tf	332.15	K	Polymorphism of gemfibrozil: Investigation by thermal and spectroscopic methods
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.27	J/mol×K	744.48	Joback Method

cpg	623.18	J/mol×K	777.63	Joback Method
cpg	636.24	J/mol×K	810.78	Joback Method
cpg	648.49	J/mol×K	843.94	Joback Method
cpg	659.95	J/mol×K	877.09	Joback Method
cpg	670.67	J/mol×K	910.24	Joback Method
cpg	680.69	J/mol×K	943.39	Joback Method
dvisc	0.0008477	Pa×s	445.67	Joback Method
dvisc	0.0003453	Pa×s	495.47	Joback Method
dvisc	0.0001657	Pa×s	545.27	Joback Method
dvisc	0.0000899	Pa×s	595.08	Joback Method
dvisc	0.0000536	Pa×s	644.88	Joback Method
dvisc	0.0000345	Pa×s	694.68	Joback Method
dvisc	0.0000235	Pa×s	744.48	Joback Method

Sources

Polymorphism of gemfibrozil: Investigation by thermal and spectroscopic methods: https://www.doi.org/10.1016/j.tca.2019.03.026

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=C25812300&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
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume