

Fenbufen, hydroxy, bis-methylated

Inchi:	InChI=1S/C18H18O4/c1-21-16-9-7-14(8-10-16)13-3-5-15(6-4-13)17(19)11-12-18(20)22-2
InchiKey:	PGZCTHBBQUEDCY-UHFFFAOYSA-N
Formula:	C18H18O4
SMILES:	<chem>COC(=O)CCC(=O)c1ccc(-c2ccc(OC)cc2)cc1</chem>
Mol. weight [g/mol]:	298.33

Physical Properties

Property code	Value	Unit	Source
gf	-161.60	kJ/mol	Joback Method
hf	-454.33	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.498		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinsol	2190.00		NIST Webbook
tb	827.14	K	Joback Method
tc	1056.49	K	Joback Method
tf	514.82	K	Joback Method
vc	0.875	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.96	J/molxK	827.14	Joback Method
cpg	724.04	J/molxK	1018.26	Joback Method
cpg	715.01	J/molxK	980.04	Joback Method
cpg	704.81	J/molxK	941.81	Joback Method
cpg	693.42	J/molxK	903.59	Joback Method
cpg	680.81	J/molxK	865.36	Joback Method
cpg	731.93	J/molxK	1056.49	Joback Method
dvisc	0.0000743	Paxs	827.14	Joback Method
dvisc	0.0000925	Paxs	775.09	Joback Method

dvisc	0.0001189	Paxs	723.03	Joback Method
dvisc	0.0001590	Paxs	670.98	Joback Method
dvisc	0.0002232	Paxs	618.93	Joback Method
dvisc	0.0003335	Paxs	566.87	Joback Method
dvisc	0.0005404	Paxs	514.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201586&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
mvol:	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

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