Fenbufen methyl derivative

Other names: Fenbufen, methylated
Methyl 4-oxo-4-(4-phenylphenyl)butanoate
Inchi: InChI=1S/C17H16O3/c1-20-17(19)12-11-16(18)15-9-7-14(8-10-15)13-5-3-2-4-6-13/h2-10
InchiKey: NHEVNQGUSJUPBZ-UHFFFAOYSA-N
Formula: C17H16O3
SMILES: COC(=O)CCC(=O)c1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 268.31
CAS: 54011-27-7

Physical Properties

Property code	Value	Unit	Source
gf	-55.39	kJ/mol	Joback Method
hf	-290.00	kJ/mol	Joback Method
hfus	31.86	kJ/mol	Joback Method
hvap	74.55	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.490		Crippen Method
mcvol	211.880	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	776.86	K	Joback Method
tc	1011.64	K	Joback Method
tf	468.80	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.59	J/mol×K	776.86	Joback Method
cpg	646.55	J/mol×K	972.51	Joback Method
cpg	636.77	J/mol×K	933.38	Joback Method
cpg	625.93	J/mol×K	894.25	Joback Method
cpg	613.99	J/mol×K	855.12	Joback Method

cpg	600.89	J/mol×K	815.99	Joback Method
cpg	655.33	J/mol×K	1011.64	Joback Method
dvisc	0.0001090	Pa×s	776.86	Joback Method
dvisc	0.0001375	Pa×s	725.52	Joback Method
dvisc	0.0001795	Pa×s	674.17	Joback Method
dvisc	0.0002449	Pa×s	622.83	Joback Method
dvisc	0.0003533	Pa×s	571.49	Joback Method
dvisc	0.0005480	Pa×s	520.14	Joback Method
dvisc	0.0009357	Pa×s	468.80	Joback Method

Sources

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=C54011277&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume