Fenbufen

Other names: 3-(4-Biphenylcarbonyl)propionic acid
3-(4-Biphenylylcarbonyl)propionic acid
3-(4-Biphenylylcarbonyl)propionic acid (fenbufen)
3-(4-Phenylbenzoyl)propionic acid
4-(4-Biphenylyl)-4-oxobutyric acid
Bufemid
Butyric acid 4-(4-biphenyl)-4-oxo-
CL 82204
Cinopal
Cinopol
Diphenyl-4-«gamma»-oxo-«gamma»-butyric acid
Diphenyl-4-Â«gammaÂ»-oxo-Â«gammaÂ»-butyric acid
Lederfen
Napanol
Propionic acid, 3-(4-biphenylylcarbonyl)-
[1,1'-Biphenyl]-4-butanoic acid, «gamma»-oxo-
[1,1'-Biphenyl]-4-butanoic acid, Â«gammaÂ»-oxo-
«beta»,p-Phenylbenzoylpropionic acid
«gamma»-Oxo(1,1'-biphenyl)-4-butanoic acid
Â«betaÂ»,p-Phenylbenzoylpropionic acid
Â«gammaÂ»-Oxo(1,1'-biphenyl)-4-butanoic acid

Inchi: InChI=1S/C16H14O3/c17-15(10-11-16(18)19)14-8-6-13(7-9-14)12-4-2-1-3-5-12/h1-9H,10

InchiKey: ZPAKPRAICRBAOD-UHFFFAOYSA-N

Formula: C16H14O3

SMILES: O=C(O)CCC(=O)c1ccc(-c2ccccc2)cc1

Mol. weight [g/mol]: 254.28

CAS: 36330-85-5

Physical Properties

Property code	Value	Unit	Source
gf	-95.63	kJ/mol	Joback Method
hf	-289.37	kJ/mol	Joback Method
hfus	32.17	kJ/mol	Joback Method
hsub	154.90 ± 0.80	kJ/mol	NIST Webbook
hvap	86.59	kJ/mol	Joback Method

log10ws	-5.30		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-4.53		Aqueous Solubility Prediction Method
logp	3.401		Crippen Method
mcvol	197.790	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	823.74	K	Joback Method
tc	1049.14	K	Joback Method
tf	459.18	K	Aqueous Solubility Prediction Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.50	J/mol×K	823.74	Joback Method
cpg	567.66	J/mol×K	861.31	Joback Method
cpg	577.91	J/mol×K	898.87	Joback Method
cpg	587.30	J/mol×K	936.44	Joback Method
cpg	595.89	J/mol×K	974.01	Joback Method
cpg	603.75	J/mol×K	1011.57	Joback Method
cpg	610.94	J/mol×K	1049.14	Joback Method
dvisc	0.0003170	Pa×s	550.72	Joback Method
dvisc	0.0007115	Pa×s	496.12	Joback Method
dvisc	0.0001635	Pa×s	605.33	Joback Method
dvisc	0.0000940	Pa×s	659.93	Joback Method
dvisc	0.0000589	Pa×s	714.53	Joback Method
dvisc	0.0000394	Pa×s	769.14	Joback Method
dvisc	0.0000278	Pa×s	823.74	Joback Method
hfust	41.10	kJ/mol	462.90	NIST Webbook
hfust	46.20	kJ/mol	459.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C36330855&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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
hsub:	Enthalpy of sublimation 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