Bifenazate

Other names: Hydrazinecarboxylic acid, 2-(4-methoxy[1,1'-biphenyl]-3-yl)-, 1-methylethyl ester
Inchi: InChI=1S/C17H20N2O3/c1-12(2)22-17(20)19-18-15-11-14(9-10-16(15)21-3)13-7-5-4-6-8
InchiKey: VHLKTXFWDRXILV-UHFFFAOYSA-N
Formula: C17H20N2O3
SMILES: COc1ccc(-c2ccccc2)cc1NNC(=O)OC(C)C
Mol. weight [g/mol]: 300.35
CAS: 149877-41-8

Physical Properties

Property code	Value	Unit	Source
gf	135.24	kJ/mol	Joback Method
hf	-219.45	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	83.36	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	3.824		Crippen Method
mcvol	236.140	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	2515.20		NIST Webbook
tb	850.29	K	Joback Method
tc	1079.36	K	Joback Method
tf	543.94	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.66	J/mol×K	850.29	Joback Method
cpg	720.46	J/mol×K	888.47	Joback Method
cpg	732.99	J/mol×K	926.65	Joback Method
cpg	744.27	J/mol×K	964.83	Joback Method
cpg	754.33	J/mol×K	1003.01	Joback Method
cpg	763.21	J/mol×K	1041.18	Joback Method
cpg	770.94	J/mol×K	1079.36	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C149877418&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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