Mepronil

Other names: Basitac
Benzamide, 2-methyl-N-(3-(1-methylethoxy)phenyl)-
3'-Isopropoxy-2-methylbenzanilide
2-Methyl-N-(3-(1-methylethoxy)phenyl)benzamide
Inchi: InChI=1S/C17H19NO2/c1-12(2)20-15-9-6-8-14(11-15)18-17(19)16-10-5-4-7-13(16)3/h4-
InchiKey: BCTQJXQXJVLSIG-UHFFFAOYSA-N
Formula: C17H19NO2
SMILES: Cc1ccccc1C(=O)Nc1cccc(OC(C)C)c1
Mol. weight [g/mol]: 269.34
CAS: 55814-41-0

Physical Properties

Property code	Value	Unit	Source
gf	150.85	kJ/mol	Joback Method
hf	-140.70	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	74.52	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.035		Crippen Method
mcvol	220.290	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	2308.00		NIST Webbook
rinpol	2298.00		NIST Webbook
rinpol	2298.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	777.70	K	Joback Method
tc	1010.20	K	Joback Method
tf	469.05	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.49	J/mol×K	777.70	Joback Method

cpg	640.95	J/mol×K	816.45	Joback Method
cpg	655.18	J/mol×K	855.20	Joback Method
cpg	668.21	J/mol×K	893.95	Joback Method
cpg	680.10	J/mol×K	932.70	Joback Method
cpg	690.90	J/mol×K	971.45	Joback Method
cpg	700.66	J/mol×K	1010.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C55814410&Units=SI

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