dimetan

Inchi: InChI=1S/C11H17NO3/c1-11(2)6-8(13)5-9(7-11)15-10(14)12(3)4/h5H,6-7H2,1-4H3
InchiKey: ITEQSCBLCCNACE-UHFFFAOYSA-N
Formula: C11H17NO3
SMILES: CN(C)C(=O)OC1=CC(=O)CC(C)(C)C1
Mol. weight [g/mol]: 211.26

Physical Properties

Property code	Value	Unit	Source
gf	-164.70	kJ/mol	Joback Method
hf	-469.47	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	55.76	kJ/mol	Joback Method
log10ws	-0.85		Aqueous Solubility Prediction Method
log10ws	-0.85		Estimated Solubility Method
logp	1.958		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	631.56	K	Joback Method
tc	854.85	K	Joback Method
tf	318.65	K	Aqueous Solubility Prediction Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.60	J/mol×K	631.56	Joback Method
cpg	469.31	J/mol×K	668.77	Joback Method
cpg	485.15	J/mol×K	705.99	Joback Method
cpg	500.21	J/mol×K	743.20	Joback Method
cpg	514.58	J/mol×K	780.42	Joback Method
cpg	528.33	J/mol×K	817.63	Joback Method
cpg	541.54	J/mol×K	854.85	Joback Method

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume