4-Methyl-n-(3-oxo-1,3-dihydro-2-benzofuran-1-yl)b

Inchi: InChI=1S/C15H13NO4S/c1-10-6-8-11(9-7-10)21(18,19)16-14-12-4-2-3-5-13(12)15(17)20
InchiKey: HRDCLCAHDMYEJB-UHFFFAOYSA-N
Formula: C15H13NO4S
SMILES: Cc1ccc(S(=O)(=O)NC2OC(=O)c3ccccc32)cc1
Mol. weight [g/mol]: 303.33
CAS: 101097-83-0

Physical Properties

Property code	Value	Unit	Source
gf	-246.13	kJ/mol	Joback Method
hf	-499.59	kJ/mol	Joback Method
hfus	44.01	kJ/mol	Joback Method
hvap	88.60	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	2.143		Crippen Method
mcvol	209.340	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	805.38	K	Joback Method
tc	1051.28	K	Joback Method
tf	540.64	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.30	J/mol×K	805.38	Joback Method
cpg	615.94	J/mol×K	846.36	Joback Method
cpg	628.14	J/mol×K	887.35	Joback Method
cpg	638.94	J/mol×K	928.33	Joback Method
cpg	648.38	J/mol×K	969.32	Joback Method
cpg	656.49	J/mol×K	1010.30	Joback Method
cpg	663.31	J/mol×K	1051.28	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=C101097830&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
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

Latest version available from:
https://www.chemeo.com/cid/11-646-2/4-Methyl-n-3-oxo-1-3-dihydro-2-benzofuran-1-yl-benzenesulfonamide.pdf
Generated by Cheméo on 2024-05-02 22:29:06.028428663 +0000 UTC m=+16978194.949005995.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.