Benfuresate

Other names: 2,3-dihydro-3,3-dimethyl-5-benzofurylethanesulphonate
Inchi: InChI=1S/C12H16O4S/c1-4-17(13,14)16-9-5-6-11-10(7-9)12(2,3)8-15-11/h5-7H,4,8H2,1-
InchiKey: QGQSRQPXXMTJCM-UHFFFAOYSA-N
Formula: C12H16O4S
SMILES: CCS(=O)(=O)Oc1ccc2c(c1)C(C)(C)CO2
Mol. weight [g/mol]: 256.32
CAS: 68505-69-1

Physical Properties

Property code	Value	Unit	Source
gf	-461.09	kJ/mol	Joback Method
hf	-706.95	kJ/mol	Joback Method
hfus	32.48	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.085		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	1871.00		NIST Webbook
tb	614.73	K	Joback Method
tc	827.86	K	Joback Method
tf	405.66	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.65	J/mol×K	614.73	Joback Method
cpg	488.03	J/mol×K	650.25	Joback Method
cpg	502.52	J/mol×K	685.77	Joback Method
cpg	516.23	J/mol×K	721.30	Joback Method
cpg	529.26	J/mol×K	756.82	Joback Method
cpg	541.70	J/mol×K	792.34	Joback Method
cpg	553.66	J/mol×K	827.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68505691&Units=SI
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

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

Latest version available from:
https://www.chemeo.com/cid/50-167-1/Benfuresate.pdf
Generated by Cheméo on 2025-12-05 22:32:56.199331097 +0000 UTC m=+4722173.729371752.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.