Bicyclo[3.2.1]octane-2,3,4-trione

Inchi: InChI=1S/C8H8O3/c9-6-4-1-2-5(3-4)7(10)8(6)11/h4-5H,1-3H2
InchiKey: VZAMUQOALSICKQ-UHFFFAOYSA-N
Formula: C8H8O3
SMILES: O=C1C(=O)C2CCC(C2)C1=O
Mol. weight [g/mol]: 152.15
CAS: 25352-00-5

Physical Properties

Property code	Value	Unit	Source
gf	-253.99	kJ/mol	Joback Method
hf	-488.27	kJ/mol	Joback Method
hfus	7.08	kJ/mol	Joback Method
hvap	46.31	kJ/mol	Joback Method
ie	9.49	eV	NIST Webbook
log10ws	-0.32		Crippen Method
logp	0.124		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
tb	607.92	K	Joback Method
tc	869.42	K	Joback Method
tf	413.42	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.28	J/mol×K	607.92	Joback Method
cpg	303.38	J/mol×K	651.50	Joback Method
cpg	318.50	J/mol×K	695.09	Joback Method
cpg	332.60	J/mol×K	738.67	Joback Method
cpg	345.63	J/mol×K	782.25	Joback Method
cpg	357.51	J/mol×K	825.84	Joback Method
cpg	368.20	J/mol×K	869.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25352005&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

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
ie:	Ionization energy
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