BICYCLO[4.2.0]OCTA-1,3,5-TRIENE-7,8-DIONE

Inchi: InChI=1S/C8H4O2/c9-7-5-3-1-2-4-6(5)8(7)10/h1-4H
InchiKey: NFYYUUJYMWILSY-UHFFFAOYSA-N
Formula: C8H4O2
SMILES: O=c1c(=O)c2ccccc12
Mol. weight [g/mol]: 132.12

Physical Properties

Property code	Value	Unit	Source
hf	-77.01	kJ/mol	Cheméo Relay (1.0)
hvap	68.44	kJ/mol	Cheméo Relay (1.0)
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-2.13		Cheméo Relay (1.0)
logp	0.436		Crippen Method
mcvol	92.100	ml/mol	McGowan Method
pc	3938.24	kPa	Cheméo Relay (1.0, beta)
tb	533.21	K	Cheméo Relay (1.0)
tc	791.39	K	Cheméo Relay (1.0)
tf	419.97	K	Cheméo Relay (1.0)
vc	0.350	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6383115&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

hf:	Enthalpy of formation 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