2-(2-oxoethyl)-cis-Bicyclo[3.3.0]octane-3,7-dione

Inchi: InChI=1S/C10H12O3/c11-2-1-8-9-5-7(12)3-6(9)4-10(8)13/h2,6,8-9H,1,3-5H2/t6-,8?,9-/m1
InchiKey: DIBJWGBHNVSLPK-CQTSCFDVSA-N
Formula: C10H12O3
SMILES: O=CCC1C(=O)CC2CC(=O)CC21
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
gf	-221.79	kJ/mol	Joback Method
hf	-497.77	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	52.93	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	0.760		Crippen Method
mcvol	134.750	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	1734.00		NIST Webbook
tb	629.85	K	Joback Method
tc	868.25	K	Joback Method
tf	405.50	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.92	J/mol×K	629.85	Joback Method
cpg	395.73	J/mol×K	669.58	Joback Method
cpg	411.48	J/mol×K	709.32	Joback Method
cpg	426.15	J/mol×K	749.05	Joback Method
cpg	439.76	J/mol×K	788.79	Joback Method
cpg	452.30	J/mol×K	828.52	Joback Method
cpg	463.75	J/mol×K	868.25	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=R419153&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume