Syn-tricyclo[6.2.0.03,6]decane-2,7-dione

Inchi: InChI=1S/C10H12O2/c11-9-5-1-2-6(5)10(12)8-4-3-7(8)9/h5-8H,1-4H2/t5-,6+,7+,8-
InchiKey: XVOUTQMRFQTWOB-SOSBWXJGSA-N
Formula: C10H12O2
SMILES: O=C1C2CCC2C(=O)C2CCC12
Mol. weight [g/mol]: 164.20
CAS: 87305-43-9

Physical Properties

Property code	Value	Unit	Source
gf	-49.42	kJ/mol	Joback Method
hf	-333.23	kJ/mol	Joback Method
hfus	14.05	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-1.29		Crippen Method
logp	1.191		Crippen Method
mcvol	122.320	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	583.66	K	Joback Method
tc	829.88	K	Joback Method
tf	384.96	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.99	J/mol×K	583.66	Joback Method
cpg	361.57	J/mol×K	624.70	Joback Method
cpg	378.93	J/mol×K	665.73	Joback Method
cpg	395.12	J/mol×K	706.77	Joback Method
cpg	410.19	J/mol×K	747.81	Joback Method
cpg	424.18	J/mol×K	788.85	Joback Method
cpg	437.16	J/mol×K	829.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87305439&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