

Tricyclo[4.2.1.0^{2,5}]nonane-3,4-dione, anti-

Inchi:	InChI=1S/C9H10O2/c10-8-6-4-1-2-5(3-4)7(6)9(8)11/h4-7H,1-3H2/t4-,5-,6-,7+/m1/s1
InchiKey:	ORYDRYMEZOIOGV-GBNDHIKLSA-N
Formula:	C9H10O2
SMILES:	O=C1C(=O)C2C3CCC(C3)C12
Mol. weight [g/mol]:	150.17
CAS:	67843-61-2

Physical Properties

Property code	Value	Unit	Source
gf	-45.74	kJ/mol	Joback Method
hf	-306.43	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	43.55	kJ/mol	Joback Method
ie	8.85	eV	NIST Webbook
log10ws	-0.87		Crippen Method
logp	0.801		Crippen Method
mcvol	108.230	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	556.51	K	Joback Method
tc	799.05	K	Joback Method
tf	377.21	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.08	J/mol×K	556.51	Joback Method
cpg	310.86	J/mol×K	596.93	Joback Method
cpg	326.56	J/mol×K	637.36	Joback Method
cpg	341.23	J/mol×K	677.78	Joback Method
cpg	354.92	J/mol×K	718.20	Joback Method
cpg	367.69	J/mol×K	758.62	Joback Method
cpg	379.58	J/mol×K	799.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67843612&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

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