

Pentacyclo[5.4.0.0(2,6).0(3,10).0(5,9)]undecane-8,11-dione

Other names:	Pentacyclo[5.4.0.02,6.03,10.05,9]undecan-8,11-dione Pentacyclo[5.4.0.0
Inchi:	InChI=1S/C11H10O2/c12-10-6-2-1-3-5-4(2)8(10)9(5)11(13)7(3)6/h2-9H,1H2
InchiKey:	WTUFOKOJVXNYTJ-UHFFFAOYSA-N
Formula:	C11H10O2
SMILES:	O=C1C2C3CC4C2C(=O)C2C1C3C42
Mol. weight [g/mol]:	174.20
CAS:	2958-72-7

Physical Properties

Property code	Value	Unit	Source
chs	-5559.57	kJ/mol	NIST Webbook
gf	125.58	kJ/mol	Joback Method
hf	-218.15	kJ/mol	Joback Method
hfs	-198.30	kJ/mol	NIST Webbook
hfus	25.55	kJ/mol	Joback Method
hsub	92.60 ± 1.00	kJ/mol	NIST Webbook
hvap	46.52	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
log10ws	-0.53		Crippen Method
logp	0.512		Crippen Method
mcvol	114.690	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
tb	589.33	K	Joback Method
tc	823.53	K	Joback Method
tf	441.23	K	Joback Method
tt	516.80 ± 2.00	K	NIST Webbook
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.82	J/molxK	589.33	Joback Method
cpg	377.56	J/molxK	628.36	Joback Method

cpg	393.06	J/mol×K	667.40	Joback Method
cpg	407.48	J/mol×K	706.43	Joback Method
cpg	420.97	J/mol×K	745.46	Joback Method
cpg	433.68	J/mol×K	784.49	Joback Method
cpg	445.76	J/mol×K	823.53	Joback Method
hfust	5.23	kJ/mol	516.80	NIST Webbook
hfust	3.94	kJ/mol	516.80	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C2958727&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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