Octahydro-1,3,6-ethanylylidenecyclobuta [cd] indene-2,8(1H)-dione

Inchi: InChI=1S/C12H12O2/c13-11-7-3-1-2-4-6-5(3)9(11)10(6)12(14)8(4)7/h3-10H,1-2H2
InchiKey: QKFUKYWULIYZFN-UHFFFAOYSA-N
Formula: C12H12O2
SMILES: O=C1C2C3CCC4C2C(=O)C2C1C3C42
Mol. weight [g/mol]: 188.22
CAS: 712-25-4

Physical Properties

Property code	Value	Unit	Source
chs	-6197.76	kJ/mol	NIST Webbook
gf	121.90	kJ/mol	Joback Method
hf	-244.95	kJ/mol	Joback Method
hfs	-239.50	kJ/mol	NIST Webbook
hfus	26.04	kJ/mol	Joback Method
hvap	48.92	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	0.902		Crippen Method
mcvol	128.780	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	616.48	K	Joback Method
tc	853.99	K	Joback Method
tf	448.98	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.96	J/mol×K	616.48	Joback Method
cpg	430.15	J/mol×K	656.07	Joback Method
cpg	447.05	J/mol×K	695.65	Joback Method
cpg	462.80	J/mol×K	735.24	Joback Method
cpg	477.56	J/mol×K	774.82	Joback Method
cpg	491.47	J/mol×K	814.41	Joback Method
cpg	504.70	J/mol×K	853.99	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C712254&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume