

endo-(2s,7R)-Tricyclo[6.2.2.0(2,7)]-4,9-dodecadien

Other names:	Endo-1,4a,8,8a-tetrahydro-1,4-ethanonaphthalene-5,8-dione
Inchi:	InChI=1S/C12H12O2/c13-9-5-6-10(14)12-8-2-1-7(3-4-8)11(9)12/h1-2,5-8,11-12H,3-4H2
InchiKey:	RVYRSLQPTCIBMM-UHFFFAOYSA-N
Formula:	C12H12O2
SMILES:	O=C1C=CC(=O)C2C3C=CC(CC3)C12
Mol. weight [g/mol]:	188.22
CAS:	2816-25-3

Physical Properties

Property code	Value	Unit	Source
chs	-6215.30	kJ/mol	NIST Webbook
gf	3.14	kJ/mol	Joback Method
hf	-271.27	kJ/mol	Joback Method
hfs	-222.00	kJ/mol	NIST Webbook
hfus	17.48	kJ/mol	Joback Method
hvap	51.33	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.523		Crippen Method
mcvol	141.900	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	636.28	K	Joback Method
tc	893.95	K	Joback Method
tf	401.98	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.22	J/molxK	636.28	Joback Method
cpg	423.53	J/molxK	679.22	Joback Method
cpg	441.40	J/molxK	722.17	Joback Method
cpg	457.87	J/molxK	765.11	Joback Method
cpg	473.00	J/molxK	808.06	Joback Method
cpg	486.82	J/molxK	851.00	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2816253&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

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