4,7-Methano-1H-isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-, (3a«alpha»,4«alpha»,7«alpha»,7a«alpha»)-

Other names: 5-Norbornene-2,3-dicarboximide, cis-endo-; 5-Norbornene-endo-2,3-dicarboximide

Inchi: InChI=1S/C9H9NO2/c11-8-6-4-1-2-5(3-4)7(6)9(12)10-8/h1-2,4-7H,3H2,(H,10,11,12)

InchiKey: GPIUUMROPXDNRH-UHFFFAOYSA-N

Formula: C9H9NO2

SMILES: O=C1NC(=O)C2C3C=CC(C3)C12

Mol. weight [g/mol]: 163.17

CAS: 6265-30-1

Physical Properties

Property code	Value	Unit	Source
gf	59.83	kJ/mol	Joback Method
hf	-217.00	kJ/mol	Joback Method
hfus	22.27	kJ/mol	Joback Method
hvap	50.77	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.081		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
tb	608.49	K	Joback Method
tc	865.69	K	Joback Method
tf	454.00 ± 2.00	K	NIST Webbook
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.10	J/mol×K	608.49	Joback Method
cpg	334.48	J/mol×K	651.36	Joback Method
cpg	349.74	J/mol×K	694.22	Joback Method
cpg	363.92	J/mol×K	737.09	Joback Method
cpg	377.06	J/mol×K	779.95	Joback Method
cpg	389.19	J/mol×K	822.82	Joback Method
cpg	400.35	J/mol×K	865.69	Joback Method

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=C6265301&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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