Exo-4-hydroxy-exo-endo-tetracyclo[6.2.1.13,602,7

Other names: Exo-4-hydroxy-exo-endo-tetracyclo[6.2.1.1
Inchi: InChI=1S/C12H18O/c13-10-5-8-4-9(10)12-7-2-1-6(3-7)11(8)12/h6-13H,1-5H2/t6-,7+,8+,9
InchiKey: LXGJTVCALLQHGZ-IGADDSOASA-N
Formula: C12H18O
SMILES: OC1CC2CC1C1C3CCC(C3)C21
Mol. weight [g/mol]: 178.27
CAS: 107133-43-7

Physical Properties

Property code	Value	Unit	Source
chs	-7000.30 ± 4.60	kJ/mol	NIST Webbook
gf	133.21	kJ/mol	Joback Method
hf	-218.00 ± 5.00	kJ/mol	NIST Webbook
hfs	-294.30 ± 4.60	kJ/mol	NIST Webbook
hfus	26.68	kJ/mol	Joback Method
hsub	76.30	kJ/mol	NIST Webbook
hsub	76.30 ± 2.00	kJ/mol	NIST Webbook
hsub	76.30 ± 2.00	kJ/mol	NIST Webbook
hvap	57.71	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.049		Crippen Method
mcvol	142.370	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
tb	579.09	K	Joback Method
tc	780.15	K	Joback Method
tf	344.86	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.07	J/mol×K	579.09	Joback Method
cpg	445.44	J/mol×K	612.60	Joback Method
cpg	462.60	J/mol×K	646.11	Joback Method

cpg	478.65	J/mol×K	679.62	Joback Method
cpg	493.69	J/mol×K	713.13	Joback Method
cpg	507.83	J/mol×K	746.64	Joback Method
cpg	521.17	J/mol×K	780.15	Joback Method
dvisc	0.0050743	Pa×s	344.86	Joback Method
dvisc	0.0045720	Pa×s	383.90	Joback Method
dvisc	0.0041994	Pa×s	422.94	Joback Method
dvisc	0.0039131	Pa×s	461.98	Joback Method
dvisc	0.0036866	Pa×s	501.01	Joback Method
dvisc	0.0035032	Pa×s	540.05	Joback Method
dvisc	0.0033520	Pa×s	579.09	Joback Method
hsubt	74.30 ± 1.80	kJ/mol	338.00	NIST Webbook

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=C107133437&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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