1,4-Cyclohexanedione bis(ethylene ketal)

Other names: 1,4,9,12-Tetraoxadispiro(4.2.4.2)tetradecane
Inchi: InChI=1S/C10H16O4/c1-2-10(13-7-8-14-10)4-3-9(1)11-5-6-12-9/h1-8H2
InchiKey: YSMVSEYPOBXSOK-UHFFFAOYSA-N
Formula: C10H16O4
SMILES: C1COC2(CCC3(CC2)OCCO3)O1
Mol. weight [g/mol]: 200.23
CAS: 183-97-1

Physical Properties

Property code	Value	Unit	Source
gf	-192.68	kJ/mol	Joback Method
hf	-539.31	kJ/mol	Joback Method
hfus	23.81	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.047		Crippen Method
mcvol	142.660	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	582.72	K	Joback Method
tc	843.48	K	Joback Method
tf	350.00 ± 1.00	K	NIST Webbook
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.60	J/mol×K	582.72	Joback Method
cpg	424.14	J/mol×K	626.18	Joback Method
cpg	442.07	J/mol×K	669.64	Joback Method
cpg	458.81	J/mol×K	713.10	Joback Method
cpg	474.78	J/mol×K	756.56	Joback Method
cpg	490.39	J/mol×K	800.02	Joback Method
cpg	506.06	J/mol×K	843.48	Joback Method
hfust	25.77	kJ/mol	353.20	NIST Webbook

hfust	25.77	kJ/mol	353.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	0.07	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=C183971&Units=SI

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
hfust:	Enthalpy of fusion 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume