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

Physical Properties

Property code	Value	Unit	Source
hfus	23.81	kJ/mol	Joback Method
hvap	67.68	kJ/mol	Cheméo Relay (1.0)
ie	8.96	eV	Cheméo Relay (1.0)
logp	1.047		Crippen Method
mcvol	142.660	ml/mol	McGowan Method
tf	350.00 ± 1.00	K	NIST Webbook

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C183971&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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