1,10-Cycloeicosanedione

Inchi: InChI=1S/C20H36O2/c21-19-15-11-7-3-1-2-4-8-12-16-20(22)18-14-10-6-5-9-13-17-19/h1
InchiKey: LDGQUFYTSFGKFE-UHFFFAOYSA-N
Formula: C20H36O2
SMILES: O=C1CCCCCCCCCCC(=O)CCCCCCCC1
Mol. weight [g/mol]: 308.50
CAS: 14113-56-5

Physical Properties

Property code	Value	Unit	Source
gf	-264.90	kJ/mol	Joback Method
hf	-743.11	kJ/mol	Joback Method
hfus	7.94	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.160		Crippen Method
mcvol	284.940	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
tb	876.64	K	Joback Method
tc	1158.91	K	Joback Method
tf	413.94	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.23	J/mol×K	876.64	Joback Method
cpg	1021.82	J/mol×K	923.68	Joback Method
cpg	1042.48	J/mol×K	970.73	Joback Method
cpg	1057.95	J/mol×K	1017.77	Joback Method
cpg	1068.02	J/mol×K	1064.82	Joback Method
cpg	1072.43	J/mol×K	1111.86	Joback Method
cpg	1070.95	J/mol×K	1158.91	Joback Method
hfust	55.06	kJ/mol	327.20	NIST Webbook
hfust	55.06	kJ/mol	327.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14113565&Units=SI
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume