

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/h1-20
InchiKey: LDGQUFYTSFGKFE-UHFFFAOYSA-N
Formula: C20H36O2
SMILES: O=C1CCCCCCCCCCC(=O)CCCCCCCC1
Mol. weight [g/mol]: 308.51

Physical Properties

Property code	Value	Unit	Source
af	0.4553		Cheméo Relay (1.0)
gf	-264.90	kJ/mol	Joback Method
hf	-691.47	kJ/mol	Cheméo Relay (1.0)
hfus	7.94	kJ/mol	Joback Method
hvap	97.03	kJ/mol	Cheméo Relay (1.0)
ie	8.71	eV	Cheméo Relay (1.0)
log10ws	-4.95		Cheméo Relay (1.0)
logp	6.160		Crippen Method
mcvol	284.940	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
tb	700.21	K	Cheméo Relay (1.0)
tc	903.53	K	Cheméo Relay (1.0)
tf	371.54	K	Cheméo Relay (1.0)
vc	0.890	m3/kmol	Cheméo Relay (1.0)

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

Sources

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=C14113565&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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