

Cyclohexanehexanoic acid, e,2-dioxo-, methyl ester

Inchi:	InChI=1S/C13H20O4/c1-17-13(16)9-5-4-8-12(15)10-6-2-3-7-11(10)14/h14H,2-9H2,1H3
InchiKey:	INHIKRKQOXBOM-UHFFFAOYSA-N
Formula:	C13H20O4
SMILES:	COC(=O)CCCCC(=O)C1=C(O)CCCC1
Mol. weight [g/mol]:	240.30

Physical Properties

Property code	Value	Unit	Source
gf	-398.22	kJ/mol	Joback Method
hf	-711.76	kJ/mol	Joback Method
hfus	29.11	kJ/mol	Joback Method
hvap	79.47	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.675		Crippen Method
mcvol	193.750	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
tb	752.52	K	Joback Method
tc	950.08	K	Joback Method
tf	456.60	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.33	J/molxK	752.52	Joback Method
cpg	624.42	J/molxK	917.15	Joback Method
cpg	614.41	J/molxK	884.22	Joback Method
cpg	603.60	J/molxK	851.30	Joback Method
cpg	592.00	J/molxK	818.37	Joback Method
cpg	579.58	J/molxK	785.45	Joback Method
cpg	633.67	J/molxK	950.08	Joback Method
dvisc	0.0000312	Paxs	752.52	Joback Method
dvisc	0.0000455	Paxs	703.20	Joback Method
dvisc	0.0000702	Paxs	653.88	Joback Method

dvisc	0.0001162	Paxs	604.56	Joback Method
dvisc	0.0002105	Paxs	555.24	Joback Method
dvisc	0.0004281	Paxs	505.92	Joback Method
dvisc	0.0010147	Paxs	456.60	Joback Method

Sources

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=B6008716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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

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