Hexa-1,5-diene-3,4-dione

Inchi: InChI=1S/C6H6O2/c1-3-5(7)6(8)4-2/h3-4H,1-2H2
InchiKey: MMPZYDUOPLQDHR-UHFFFAOYSA-N
Formula: C6H6O2
SMILES: C=CC(=O)C(=O)C=C
Mol. weight [g/mol]: 110.11
CAS: 104910-78-3

Physical Properties

Property code	Value	Unit	Source
gf	-82.52	kJ/mol	Joback Method
hf	-141.47	kJ/mol	Joback Method
hfus	11.93	kJ/mol	Joback Method
hvap	41.10	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
ie	9.32	eV	NIST Webbook
log10ws	-0.60		Crippen Method
logp	0.497		Crippen Method
mcvol	89.940	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	437.78	K	Joback Method
tc	635.78	K	Joback Method
tf	253.72	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.19	J/mol×K	437.78	Joback Method
cpg	170.21	J/mol×K	470.78	Joback Method
cpg	177.78	J/mol×K	503.78	Joback Method
cpg	184.93	J/mol×K	536.78	Joback Method
cpg	191.67	J/mol×K	569.78	Joback Method
cpg	198.03	J/mol×K	602.78	Joback Method
cpg	204.00	J/mol×K	635.78	Joback Method

dvisc	0.0027802	Pa×s	253.72	Joback Method
dvisc	0.0016428	Pa×s	284.40	Joback Method
dvisc	0.0010755	Pa×s	315.07	Joback Method
dvisc	0.0007591	Pa×s	345.75	Joback Method
dvisc	0.0005670	Pa×s	376.43	Joback Method
dvisc	0.0004426	Pa×s	407.10	Joback Method
dvisc	0.0003577	Pa×s	437.78	Joback Method

Sources

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=C104910783&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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