2H-Pyran-2,6(3H)-dione

Other names: Glutaconic anhydride
Inchi: InChI=1S/C5H4O3/c6-4-2-1-3-5(7)8-4/h1-2H,3H2
InchiKey: SYIUWAVTBADRJG-UHFFFAOYSA-N
Formula: C5H4O3
SMILES: O=C1C=CCC(=O)O1
Mol. weight [g/mol]: 112.08
CAS: 5926-95-4

Physical Properties

Property code	Value	Unit	Source
gf	-277.96	kJ/mol	Joback Method
hf	-421.49	kJ/mol	Joback Method
hfus	7.69	kJ/mol	Joback Method
hvap	40.76	kJ/mol	Joback Method
log10ws	-0.30		Crippen Method
logp	0.016		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	5382.80	kPa	Joback Method
ripol	2427.00		NIST Webbook
ripol	2427.00		NIST Webbook
tb	499.77	K	Joback Method
tc	751.43	K	Joback Method
tf	321.50	K	Joback Method
vc	0.271	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.06	J/mol×K	499.77	Joback Method
cpg	165.53	J/mol×K	541.71	Joback Method
cpg	175.63	J/mol×K	583.66	Joback Method
cpg	185.30	J/mol×K	625.60	Joback Method
cpg	194.48	J/mol×K	667.54	Joback Method
cpg	203.10	J/mol×K	709.48	Joback Method

cpg	211.09	J/mol×K	751.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5926954&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume