

3-Methylglutaric anhydride

Other names:	«beta»-Methylglutaric anhydride 2H-Pyran-2,6(3H)-dione, dihydro-4-methyl-
Inchi:	InChI=1S/C6H8O3/c1-4-2-5(7)9-6(8)3-4/h4H,2-3H2,1H3
InchiKey:	MGICRVTUCPFQQZ-UHFFFAOYSA-N
Formula:	C6H8O3
SMILES:	CC1CC(=O)OC(=O)C1
Mol. weight [g/mol]:	128.13
CAS:	4166-53-4

Physical Properties

Property code	Value	Unit	Source
gf	-307.21	kJ/mol	Joback Method
hf	-520.25	kJ/mol	Joback Method
hfus	10.13	kJ/mol	Joback Method
hvap	42.38	kJ/mol	Joback Method
log10ws	-0.62		Crippen Method
logp	0.486		Crippen Method
mvol	93.550	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
tb	518.82	K	Joback Method
tc	762.74	K	Joback Method
tf	327.77	K	Joback Method
vc	0.340	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.69	J/mol×K	518.82	Joback Method
cpg	229.51	J/mol×K	559.47	Joback Method
cpg	242.81	J/mol×K	600.13	Joback Method
cpg	255.52	J/mol×K	640.78	Joback Method
cpg	267.57	J/mol×K	681.44	Joback Method
cpg	278.90	J/mol×K	722.09	Joback Method
cpg	289.44	J/mol×K	762.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	454.20	K	3.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4166534&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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