3-METHYLGLUTARIC ANHYDRIDE

Other names: 2H-Pyran-2,6(3H)-dione, dihydro-4-methyl-
«beta»-Methylglutaric anhydride
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

Physical Properties

Property code	Value	Unit	Source
hf	-578.17	kJ/mol	Cheméo Relay (1.0)
hfus	10.13	kJ/mol	Joback Method
ie	11.13	eV	Cheméo Relay (1.0)
logp	0.486		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
tb	516.35	K	Cheméo Relay (1.0)
tf	317.35	K	Cheméo Relay (1.0)

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

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=C4166534&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point