3-Methyl-delta2-penten-1,5-dioic acid

Other names: 3-Methyl-delta
Inchi: InChI=1S/C6H8O4/c1-4(2-5(7)8)3-6(9)10/h2H,3H2,1H3,(H,7,8)(H,9,10)/b4-2+
InchiKey: WKRBKYFIJPGYQC-DUXPYHPUSA-N
Formula: C6H8O4
SMILES: C/C(=C\C(=O)O)CC(=O)O
Mol. weight [g/mol]: 144.13

Physical Properties

Property code	Value	Unit	Source
hfus	21.56	kJ/mol	Joback Method
ie	9.46	eV	Cheméo Relay (1.0)
logp	0.492		Crippen Method
mcvol	105.980	ml/mol	McGowan Method
pc	4910.80	kPa	Joback Method
tb	533.12	K	Cheméo Relay (1.0)
tc	753.85	K	Cheméo Relay (1.0)
tf	386.07	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.25	J/mol×K	632.82	Joback Method
cpg	261.67	J/mol×K	663.17	Joback Method
cpg	267.73	J/mol×K	693.53	Joback Method
cpg	273.46	J/mol×K	723.88	Joback Method
cpg	278.88	J/mol×K	754.23	Joback Method
cpg	283.99	J/mol×K	784.58	Joback Method
cpg	288.83	J/mol×K	814.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5746907&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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