4-METHYL HYDROGEN METHYLENESUCCINATE

Other names: 4-methyl hydrogen 2-methylenesuccinate
Butanedioic acid, methylene-, 4-methyl ester
Inchi: InChI=1S/C6H8O4/c1-4(6(8)9)3-5(7)10-2/h1,3H2,2H3,(H,8,9)
InchiKey: OIYTYGOUZOARSH-UHFFFAOYSA-N
Formula: C6H8O4
SMILES: C=C(CC(=O)OC)C(=O)O
Mol. weight [g/mol]: 144.13

Physical Properties

Property code	Value	Unit	Source
af	0.6887		Cheméo Relay (1.0)
hf	-670.47	kJ/mol	Cheméo Relay (1.0)
hfus	17.18	kJ/mol	Joback Method
hvap	73.14	kJ/mol	Cheméo Relay (1.0)
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-0.43		Cheméo Relay (1.0)
logp	0.190		Crippen Method
mcvol	105.980	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
tb	502.52	K	Cheméo Relay (1.0)
tc	692.67	K	Cheméo Relay (1.0)
tf	354.12	K	Cheméo Relay (1.0)
vc	0.381	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.60	J/mol×K	555.58	Joback Method
cpg	246.18	J/mol×K	586.54	Joback Method
cpg	253.42	J/mol×K	617.50	Joback Method
cpg	260.31	J/mol×K	648.47	Joback Method
cpg	266.86	J/mol×K	679.43	Joback Method
cpg	273.07	J/mol×K	710.39	Joback Method
cpg	278.94	J/mol×K	741.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7338274&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

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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