

Succinic acid, 2-hydroxymethylene-3-isopropylidene-, dimethyl ester

InChI: InChI=1S/C10H14O5/c1-6(2)8(10(13)15-4)7(5-11)9(12)14-3/h5,11H,1-4H3/b7-5-
InChIKey: IOLPXYDUHULVJP-ALCCZGGFSA-N

Formula: C10H14O5

SMILES: COC(=O)C(=CO)C(C(=O)OC)=C(C)C

Mol. weight [g/mol]: 214.22

Physical Properties

Property code	Value	Unit	Source
gf	-436.55	kJ/mol	Joback Method
hf	-686.49	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	73.00	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.111		Crippen Method
mvol	163.910	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	680.92	K	Joback Method
tc	874.08	K	Joback Method
tf	355.56	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.40	J/molxK	680.92	Joback Method
cpg	435.94	J/molxK	713.11	Joback Method
cpg	445.91	J/molxK	745.31	Joback Method
cpg	455.34	J/molxK	777.50	Joback Method
cpg	464.23	J/molxK	809.69	Joback Method
cpg	472.61	J/molxK	841.89	Joback Method
cpg	480.51	J/molxK	874.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000812&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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