2-Dimethylamino-methylene-3-isopropylidene succinic acid, dimethyl ester

Inchi: InChI=1S/C12H19NO4/c1-8(2)10(12(15)17-6)9(7-13(3)4)11(14)16-5/h7H,1-6H3/b9-7-

InchiKey: ONKXNLGOOGTJGA-CLFYSBASSA-N

Formula: C12H19NO4

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

Mol. weight [g/mol]: 241.28

CAS: 95533-81-6

Physical Properties

Property code	Value	Unit	Source
gf	-172.11	kJ/mol	Joback Method
hf	-508.01	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Joback Method
hvap	62.82	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.114		Crippen Method
mcvol	196.200	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
tb	646.94	K	Joback Method
tc	843.58	K	Joback Method
tf	349.75	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.92	J/mol×K	646.94	Joback Method
cpg	525.37	J/mol×K	679.71	Joback Method
cpg	539.02	J/mol×K	712.49	Joback Method
cpg	551.92	J/mol×K	745.26	Joback Method
cpg	564.08	J/mol×K	778.03	Joback Method
cpg	575.54	J/mol×K	810.81	Joback Method
cpg	586.33	J/mol×K	843.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95533816&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume