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

Inchi: InChI=1S/C14H23NO4/c1-7-18-13(16)11(9-15(5)6)12(10(3)4)14(17)19-8-2/h9H,7-8H2,1-

InchiKey: QDUVNZPXASUCLM-LUAWRHEFSA-N

Formula: C14H23NO4

SMILES: CCOC(=O)C(=CN(C)C)C(C(=O)OCC)=C(C)C

Mol. weight [g/mol]: 269.34

CAS: 97176-61-9

Physical Properties

Property code	Value	Unit	Source
gf	-155.27	kJ/mol	Joback Method
hf	-549.29	kJ/mol	Joback Method
hfus	37.08	kJ/mol	Joback Method
hvap	67.27	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.894		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
tb	692.70	K	Joback Method
tc	885.40	K	Joback Method
tf	372.29	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.37	J/mol×K	692.70	Joback Method
cpg	631.76	J/mol×K	724.82	Joback Method
cpg	646.31	J/mol×K	756.93	Joback Method
cpg	660.06	J/mol×K	789.05	Joback Method
cpg	673.04	J/mol×K	821.17	Joback Method
cpg	685.28	J/mol×K	853.28	Joback Method
cpg	696.81	J/mol×K	885.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97176619&Units=SI

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