Dimethyl-5-norbornene-2,3-dicarboxylate

Other names:	3,6-Endomethylene-«DELTA»4-tetrahydrophthalic acid dimethylester
	3,6-Endomethylene-Â«DELTAÂ»4-tetrahydrophthalic acid dimethylester
	5-Norbornene-2,3-dicarboxylic acid, dimethyl ester
	Bicyclo(2,2,1)hept-5-ene-2,3-dicarboxylic acid, dimethyl ester
	Bicyclo(2.2.1)hept-5-ene-2,3-dicarboxylic acid, dimethyl ester
	Bicyclo[2.2.1]hept-2-ene-5,6-dicarboxylic acid, dimethyl ester
	Compound 3,916
	Compound-3916
	Dimalone
	Dimelone
	Dimethyl 5-bicyclo(2.2.1)hepten-2,3-dicarboxylate
	Dimethyl bicyclo[2.2.1]-5-heptene-2,3-dicarboxylate
	Dimethyl carbate
	Dimethylester kyseliny bicyklo(2,2,1)hept-5-en-2,3-dikarboxylove
	Dimethylkarbat
	NISY
	NSC 7326
Inchi:	InChI=1S/C11H14O4/c1-14-10(12)8-6-3-4-7(5-6)9(8)11(13)15-2/h3-4,6-9H,5H2,1-2H3/t6
InchiKey:	VGQLNJWOULYVFV-WZENYGAOSA-N
Formula:	C11H14O4
SMILES:	COC(=O)C1C2C=CC(C2)C1C(=O)OC
Mol. weight [g/mol]:	210.23
CAS:	5826-73-3

Physical Properties

Property code	Value	Unit	Source
gf	-302.16	kJ/mol	Joback Method
hf	-603.43	kJ/mol	Joback Method
hfus	27.35	kJ/mol	Joback Method
hvap	58.06	kJ/mol	Joback Method
log10ws	-1.20		Aqueous Solubility Prediction Method
logp	0.771		Crippen Method
mcvol	154.710	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1413.00		NIST Webbook

rinpol	1423.00		NIST Webbook
rinpol	1434.00		NIST Webbook
tb	611.23	K	Joback Method
tc	821.35	K	Joback Method
tf	382.69	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.20	J/mol×K	611.23	Joback Method
cpg	435.68	J/mol×K	646.25	Joback Method
cpg	450.23	J/mol×K	681.27	Joback Method
cpg	463.89	J/mol×K	716.29	Joback Method
cpg	476.69	J/mol×K	751.31	Joback Method
cpg	488.65	J/mol×K	786.33	Joback Method
cpg	499.80	J/mol×K	821.35	Joback Method
dvisc	0.0020246	Pa×s	382.69	Joback Method
dvisc	0.0017265	Pa×s	420.78	Joback Method
dvisc	0.0015118	Pa×s	458.87	Joback Method
dvisc	0.0013510	Pa×s	496.96	Joback Method
dvisc	0.0012267	Pa×s	535.05	Joback Method
dvisc	0.0011283	Pa×s	573.14	Joback Method
dvisc	0.0010487	Pa×s	611.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.00 ± 1.00	K	2.70	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5826733&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume