2-Butenedioic acid (Z)-, bis(1-methylethyl) ester

Other names: Maleic acid, diisopropyl ester
2-Butenedioic acid, bis(1-methylethyl) ester
Diisopropylester kyseliny maleinove
diisopropyl maleate

Inchi: InChI=1S/C10H16O4/c1-7(2)13-9(11)5-6-10(12)14-8(3)4/h5-8H,1-4H3/b6-5-

InchiKey: FNMTVMWFISHPEV-WAYWQWQTSA-N

Formula: C10H16O4

SMILES: CC(C)OC(=O)C=CC(=O)OC(C)C

Mol. weight [g/mol]: 200.23

CAS: 10099-70-4

Physical Properties

Property code	Value	Unit	Source
gf	-359.18	kJ/mol	Joback Method
hf	-632.67	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	55.35	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.446		Crippen Method
mcvol	162.340	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
tb	584.06	K	Joback Method
tc	778.44	K	Joback Method
tf	243.00 ± 0.60	K	NIST Webbook
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.68	J/mol×K	584.06	Joback Method
cpg	409.98	J/mol×K	616.46	Joback Method
cpg	422.65	J/mol×K	648.85	Joback Method
cpg	434.69	J/mol×K	681.25	Joback Method
cpg	446.11	J/mol×K	713.65	Joback Method

cpg	456.90	J/mol×K	746.04	Joback Method
cpg	467.09	J/mol×K	778.44	Joback Method
dvisc	0.0029848	Pa×s	311.70	Joback Method
dvisc	0.0012987	Pa×s	357.09	Joback Method
dvisc	0.0006818	Pa×s	402.49	Joback Method
dvisc	0.0004078	Pa×s	447.88	Joback Method
dvisc	0.0002682	Pa×s	493.27	Joback Method
dvisc	0.0001892	Pa×s	538.67	Joback Method
dvisc	0.0001410	Pa×s	584.06	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=C10099704&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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