2-Butenedioic acid (z)-, bis(1-methylpropyl) ester

Inchi: InChI=1S/C12H20O4/c1-5-9(3)15-11(13)7-8-12(14)16-10(4)6-2/h7-10H,5-6H2,1-4H3/b8-

InchiKey: MWJNGKOBSUBRNM-FPLPWBNLSA-N

Formula: C12H20O4

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

Mol. weight [g/mol]: 228.28

CAS: 14447-12-2

Physical Properties

Property code	Value	Unit	Source
gf	-342.34	kJ/mol	Joback Method
hf	-673.95	kJ/mol	Joback Method
hfus	25.57	kJ/mol	Joback Method
hvap	59.80	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.226		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook
tb	629.82	K	Joback Method
tc	819.69	K	Joback Method
tf	334.24	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.92	J/mol×K	629.82	Joback Method
cpg	510.56	J/mol×K	661.47	Joback Method
cpg	524.47	J/mol×K	693.11	Joback Method
cpg	537.67	J/mol×K	724.76	Joback Method
cpg	550.18	J/mol×K	756.40	Joback Method
cpg	561.99	J/mol×K	788.05	Joback Method
cpg	573.11	J/mol×K	819.69	Joback Method

dvisc	0.0025822	Pa×s	334.24	Joback Method
dvisc	0.0010964	Pa×s	383.50	Joback Method
dvisc	0.0005658	Pa×s	432.77	Joback Method
dvisc	0.0003343	Pa×s	482.03	Joback Method
dvisc	0.0002177	Pa×s	531.29	Joback Method
dvisc	0.0001525	Pa×s	580.56	Joback Method
dvisc	0.0001129	Pa×s	629.82	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=C14447122&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume