PROPAN-1,3-DIOC ACID, DI[3-METHYLBUTYL] ESTER

Other names: Malonic acid, di(3-methylbutyl) ester
Inchi: InChI=1S/C13H24O4/c1-10(2)5-7-16-12(14)9-13(15)17-8-6-11(3)4/h10-11H,5-9H2,1-4H3
InchiKey: MZXKSEBRMIOIIE-UHFFFAOYSA-N
Formula: C13H24O4
SMILES: CC(C)CCOC(=O)CC(=O)OCCC(C)C
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
hf	-971.41	kJ/mol	Cheméo Relay (1.0)
hfus	27.95	kJ/mol	Joback Method
hvap	78.40	kJ/mol	Cheméo Relay (1.0)
ie	9.77	eV	Cheméo Relay (1.0)
log10ws	-3.16		Cheméo Relay (1.0)
logp	2.555		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook
tb	539.70	K	Cheméo Relay (1.0)
tc	707.89	K	Cheméo Relay (1.0)
tf	201.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.26	J/mol×K	648.54	Joback Method
cpg	652.22	J/mol×K	830.39	Joback Method
cpg	640.21	J/mol×K	800.08	Joback Method
cpg	627.48	J/mol×K	769.77	Joback Method
cpg	614.03	J/mol×K	739.46	Joback Method
cpg	599.84	J/mol×K	709.16	Joback Method
cpg	584.92	J/mol×K	678.85	Joback Method
dvisc	0.0003440	Pa×s	499.56	Joback Method

dvisc	0.0001169	Pa×s	648.54	Joback Method
dvisc	0.0001578	Pa×s	598.88	Joback Method
dvisc	0.0002249	Pa×s	549.22	Joback Method
dvisc	0.0025317	Pa×s	350.59	Joback Method
dvisc	0.0005777	Pa×s	449.91	Joback Method
dvisc	0.0011034	Pa×s	400.25	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64617965&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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