Malonic acid, isobutyl 2-methylpentyl ester

Inchi: InChI=1S/C13H24O4/c1-5-6-11(4)9-17-13(15)7-12(14)16-8-10(2)3/h10-11H,5-9H2,1-4H3
InchiKey: KRERFFOGRRCEAD-UHFFFAOYSA-N
Formula: C13H24O4
SMILES: CCCC(C)COC(=O)CC(=O)OCC(C)C
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
gf	-414.14	kJ/mol	Joback Method
hf	-811.81	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.555		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1492.00		NIST Webbook
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tb	648.54	K	Joback Method
tc	830.39	K	Joback Method
tf	350.59	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.26	J/mol×K	648.54	Joback Method
cpg	584.92	J/mol×K	678.85	Joback Method
cpg	599.84	J/mol×K	709.16	Joback Method
cpg	614.03	J/mol×K	739.46	Joback Method
cpg	627.48	J/mol×K	769.77	Joback Method
cpg	640.21	J/mol×K	800.08	Joback Method
cpg	652.22	J/mol×K	830.39	Joback Method
dvisc	0.0025317	Pa×s	350.59	Joback Method

dvisc	0.0011034	Pa×s	400.25	Joback Method
dvisc	0.0005777	Pa×s	449.91	Joback Method
dvisc	0.0003440	Pa×s	499.56	Joback Method
dvisc	0.0002249	Pa×s	549.22	Joback Method
dvisc	0.0001578	Pa×s	598.88	Joback Method
dvisc	0.0001169	Pa×s	648.54	Joback Method

Sources

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=U347866&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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