Malonic acid, isobutyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C13H24O4/c1-6-11(10(4)5)17-13(15)7-12(14)16-8-9(2)3/h9-11H,6-8H2,1-5H3
InchiKey: LRVPNPXTUVVIDQ-UHFFFAOYSA-N
Formula: C13H24O4
SMILES: CCC(OC(=O)CC(=O)OCC(C)C)C(C)C
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
gf	-416.58	kJ/mol	Joback Method
hf	-817.09	kJ/mol	Joback Method
hfus	24.43	kJ/mol	Joback Method
hvap	61.68	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.554		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
tb	648.10	K	Joback Method
tc	832.83	K	Joback Method
tf	335.59	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.70	J/mol×K	648.10	Joback Method
cpg	585.64	J/mol×K	678.89	Joback Method
cpg	600.82	J/mol×K	709.68	Joback Method
cpg	615.23	J/mol×K	740.46	Joback Method
cpg	628.87	J/mol×K	771.25	Joback Method
cpg	641.76	J/mol×K	802.04	Joback Method
cpg	653.89	J/mol×K	832.83	Joback Method
dvisc	0.0033428	Pa×s	335.59	Joback Method

dvisc	0.0012868	Pa×s	387.68	Joback Method
dvisc	0.0006210	Pa×s	439.76	Joback Method
dvisc	0.0003497	Pa×s	491.85	Joback Method
dvisc	0.0002198	Pa×s	543.93	Joback Method
dvisc	0.0001499	Pa×s	596.02	Joback Method
dvisc	0.0001087	Pa×s	648.10	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=U349046&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