Malonic acid, 2-butyl propyl ester

Inchi: InChI=1S/C10H18O4/c1-4-6-13-9(11)7-10(12)14-8(3)5-2/h8H,4-7H2,1-3H3
InchiKey: FOEGNWBVSBWKJR-UHFFFAOYSA-N
Formula: C10H18O4
SMILES: CCCOC(=O)CC(=O)OC(C)CC
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
gf	-436.96	kJ/mol	Joback Method
hf	-744.61	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	55.78	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.671		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1268.00		NIST Webbook
tb	580.34	K	Joback Method
tc	763.73	K	Joback Method
tf	331.78	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.07	J/mol×K	580.34	Joback Method
cpg	429.55	J/mol×K	610.90	Joback Method
cpg	442.48	J/mol×K	641.47	Joback Method
cpg	454.83	J/mol×K	672.03	Joback Method
cpg	466.62	J/mol×K	702.60	Joback Method
cpg	477.83	J/mol×K	733.16	Joback Method
cpg	488.46	J/mol×K	763.73	Joback Method
dvisc	0.0024229	Pa×s	331.78	Joback Method
dvisc	0.0012300	Pa×s	373.21	Joback Method

dvisc	0.0007150	Pa×s	414.63	Joback Method
dvisc	0.0004587	Pa×s	456.06	Joback Method
dvisc	0.0003168	Pa×s	497.49	Joback Method
dvisc	0.0002316	Pa×s	538.91	Joback Method
dvisc	0.0001771	Pa×s	580.34	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=U349067&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

Latest version available from:
https://www.chemeo.com/cid/68-967-4/Malonic-acid-2-butyl-propyl-ester.pdf
Generated by Cheméo on 2024-10-12 09:14:25.720766816 +0000 UTC m=+3305328.357736065.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.