Malonic acid, 3,3-dimethylbut-2-yl propyl ester

Inchi: InChI=1S/C12H22O4/c1-6-7-15-10(13)8-11(14)16-9(2)12(3,4)5/h9H,6-8H2,1-5H3
InchiKey: AEURCQIDVNSBSL-UHFFFAOYSA-N
Formula: C12H22O4
SMILES: CCCOC(=O)CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	-417.28	kJ/mol	Joback Method
hf	-794.64	kJ/mol	Joback Method
hfus	21.47	kJ/mol	Joback Method
hvap	58.93	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.308		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1402.00		NIST Webbook
tb	622.87	K	Joback Method
tc	811.82	K	Joback Method
tf	356.74	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.38	J/mol×K	622.87	Joback Method
cpg	588.77	J/mol×K	780.32	Joback Method
cpg	576.41	J/mol×K	748.83	Joback Method
cpg	563.30	J/mol×K	717.34	Joback Method
cpg	549.44	J/mol×K	685.85	Joback Method
cpg	534.80	J/mol×K	654.36	Joback Method
cpg	600.40	J/mol×K	811.82	Joback Method
dvisc	0.0001246	Pa×s	622.87	Joback Method
dvisc	0.0001685	Pa×s	578.51	Joback Method

dvisc	0.0002397	Pa×s	534.16	Joback Method
dvisc	0.0003635	Pa×s	489.81	Joback Method
dvisc	0.0005987	Pa×s	445.45	Joback Method
dvisc	0.0011014	Pa×s	401.10	Joback Method
dvisc	0.0023577	Pa×s	356.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U347201&Units=SI
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

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