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

Inchi: InChI=1S/C14H26O4/c1-6-7-8-9-17-12(15)10-13(16)18-11(2)14(3,4)5/h11H,6-10H2,1-5H
InchiKey: DQDAOMVZUXXMDW-UHFFFAOYSA-N
Formula: C14H26O4
SMILES: CCCCCOC(=O)CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 258.35

Physical Properties

Property code	Value	Unit	Source
gf	-400.44	kJ/mol	Joback Method
hf	-835.92	kJ/mol	Joback Method
hfus	26.65	kJ/mol	Joback Method
hvap	63.39	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.088		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
tb	668.63	K	Joback Method
tc	854.31	K	Joback Method
tf	379.28	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.23	J/mol×K	668.63	Joback Method
cpg	641.58	J/mol×K	699.58	Joback Method
cpg	657.08	J/mol×K	730.52	Joback Method
cpg	671.74	J/mol×K	761.47	Joback Method
cpg	685.59	J/mol×K	792.42	Joback Method
cpg	698.63	J/mol×K	823.36	Joback Method
cpg	710.90	J/mol×K	854.31	Joback Method
dvisc	0.0019390	Pa×s	379.28	Joback Method

dvisc	0.0008833	Pa×s	427.50	Joback Method
dvisc	0.0004719	Pa×s	475.73	Joback Method
dvisc	0.0002830	Pa×s	523.96	Joback Method
dvisc	0.0001849	Pa×s	572.18	Joback Method
dvisc	0.0001291	Pa×s	620.40	Joback Method
dvisc	0.0000950	Pa×s	668.63	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=U347205&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