Malonic acid, di(3,3-dimethylbut-2-yl) ester

Inchi: InChI=1S/C15H28O4/c1-10(14(3,4)5)18-12(16)9-13(17)19-11(2)15(6,7)8/h10-11H,9H2,1
InchiKey: CTNTWNUYQRQTPR-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CC(OC(=O)CC(=O)OC(C)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-391.62	kJ/mol	Joback Method
hf	-870.59	kJ/mol	Joback Method
hfus	18.31	kJ/mol	Joback Method
hvap	63.93	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.332		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
tb	687.84	K	Joback Method
tc	883.23	K	Joback Method
tf	377.97	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.96	J/mol×K	687.84	Joback Method
cpg	760.60	J/mol×K	850.66	Joback Method
cpg	746.99	J/mol×K	818.10	Joback Method
cpg	732.47	J/mol×K	785.53	Joback Method
cpg	716.98	J/mol×K	752.97	Joback Method
cpg	700.49	J/mol×K	720.40	Joback Method
cpg	773.32	J/mol×K	883.23	Joback Method
dvisc	0.0000648	Pa×s	687.84	Joback Method

dvisc	0.0000924	Pa×s	636.20	Joback Method
dvisc	0.0001405	Pa×s	584.55	Joback Method
dvisc	0.0002317	Pa×s	532.90	Joback Method
dvisc	0.0004253	Pa×s	481.26	Joback Method
dvisc	0.0009035	Pa×s	429.62	Joback Method
dvisc	0.0023579	Pa×s	377.97	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=U348670&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