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

Inchi: InChI=1S/C18H34O4/c1-13(17(3,4)5)21-15(19)11-9-10-12-16(20)22-14(2)18(6,7)8/h13-1
InchiKey: LIIWLPQEOZDNDG-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CC(OC(=O)CCCCC(=O)OC(C)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-366.36	kJ/mol	Joback Method
hf	-932.51	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	70.61	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.502		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	1885.00		NIST Webbook
tb	756.48	K	Joback Method
tc	948.35	K	Joback Method
tf	411.78	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.62	J/mol×K	756.48	Joback Method
cpg	871.84	J/mol×K	788.46	Joback Method
cpg	888.96	J/mol×K	820.44	Joback Method
cpg	905.05	J/mol×K	852.42	Joback Method
cpg	920.13	J/mol×K	884.39	Joback Method
cpg	934.27	J/mol×K	916.37	Joback Method
cpg	947.48	J/mol×K	948.35	Joback Method
dvisc	0.0015453	Pa×s	411.78	Joback Method
dvisc	0.0005795	Pa×s	469.23	Joback Method

dvisc	0.0002692	Pa×s	526.68	Joback Method
dvisc	0.0001454	Pa×s	584.13	Joback Method
dvisc	0.0000877	Pa×s	641.58	Joback Method
dvisc	0.0000575	Pa×s	699.03	Joback Method
dvisc	0.0000402	Pa×s	756.48	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=U353684&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