3-Methyladipic acid, anhydride with acetic acid

Inchi: InChI=1S/C9H14O5/c1-6(5-8(11)12)3-4-9(13)14-7(2)10/h6H,3-5H2,1-2H3,(H,11,12)
InchiKey: NBRVVWSCRRSWQW-UHFFFAOYSA-N
Formula: C9H14O5
SMILES: CC(=O)OC(=O)CCC(C)CC(=O)O
Mol. weight [g/mol]: 202.20

Physical Properties

Property code	Value	Unit	Source
gf	-606.12	kJ/mol	Joback Method
hf	-856.56	kJ/mol	Joback Method
hfus	25.62	kJ/mol	Joback Method
hvap	74.57	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	0.967		Crippen Method
mcvol	154.120	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1636.00		NIST Webbook
tb	681.09	K	Joback Method
tc	866.83	K	Joback Method
tf	409.03	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.97	J/mol×K	681.09	Joback Method
cpg	420.95	J/mol×K	712.05	Joback Method
cpg	430.39	J/mol×K	743.00	Joback Method
cpg	439.30	J/mol×K	773.96	Joback Method
cpg	447.67	J/mol×K	804.92	Joback Method
cpg	455.51	J/mol×K	835.87	Joback Method
cpg	462.83	J/mol×K	866.83	Joback Method
dvisc	0.0024732	Pa×s	409.03	Joback Method
dvisc	0.0009844	Pa×s	454.37	Joback Method

dvisc	0.0004631	Pa×s	499.72	Joback Method
dvisc	0.0002470	Pa×s	545.06	Joback Method
dvisc	0.0001451	Pa×s	590.40	Joback Method
dvisc	0.0000919	Pa×s	635.75	Joback Method
dvisc	0.0000619	Pa×s	681.09	Joback Method

Sources

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=U374904&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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