Trimethyl isocitrate

Inchi: InChI=1S/C10H16O6/c1-6(9(12)15-3)7(10(13)16-4)5-8(11)14-2/h6-7H,5H2,1-4H3
InchiKey: QJJJDRPIBYWIHG-UHFFFAOYSA-N
Formula: C10H16O6
SMILES: COC(=O)CC(C(=O)OC)C(C)C(=O)OC
Mol. weight [g/mol]: 232.23

Physical Properties

Property code	Value	Unit	Source
gf	-673.32	kJ/mol	Joback Method
hf	-994.69	kJ/mol	Joback Method
hfus	22.97	kJ/mol	Joback Method
hvap	64.55	kJ/mol	Joback Method
log10ws	-0.11		Crippen Method
logp	0.148		Crippen Method
mcvol	174.080	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	1435.00		NIST Webbook
tb	656.19	K	Joback Method
tc	849.21	K	Joback Method
tf	388.94	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.00	J/mol×K	656.19	Joback Method
cpg	472.62	J/mol×K	688.36	Joback Method
cpg	484.60	J/mol×K	720.53	Joback Method
cpg	495.91	J/mol×K	752.70	Joback Method
cpg	506.54	J/mol×K	784.87	Joback Method
cpg	516.47	J/mol×K	817.04	Joback Method
cpg	525.69	J/mol×K	849.21	Joback Method
dvisc	0.0016466	Pa×s	388.94	Joback Method
dvisc	0.0008660	Pa×s	433.48	Joback Method

dvisc	0.0005133	Pa×s	478.02	Joback Method
dvisc	0.0003327	Pa×s	522.57	Joback Method
dvisc	0.0002308	Pa×s	567.11	Joback Method
dvisc	0.0001689	Pa×s	611.65	Joback Method
dvisc	0.0001289	Pa×s	656.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R488718&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

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