Methylaconitic acid, trimethyl ester

Inchi: InChI=1S/C10H14O6/c1-6(9(12)15-3)7(10(13)16-4)5-8(11)14-2/h5H2,1-4H3/b7-6+
InchiKey: ACFSFUFJFGNCSK-VOTSOKGWSA-N
Formula: C10H14O6
SMILES: COC(=O)CC(C(=O)OC)=C(C)C(=O)OC
Mol. weight [g/mol]: 230.21

Physical Properties

Property code	Value	Unit	Source
gf	-605.32	kJ/mol	Joback Method
hf	-886.49	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Joback Method
hvap	65.44	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.212		Crippen Method
mcvol	169.780	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1428.00		NIST Webbook
tb	660.99	K	Joback Method
tc	859.91	K	Joback Method
tf	385.94	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.21	J/mol×K	660.99	Joback Method
cpg	448.06	J/mol×K	694.14	Joback Method
cpg	459.28	J/mol×K	727.30	Joback Method
cpg	469.87	J/mol×K	760.45	Joback Method
cpg	479.80	J/mol×K	793.61	Joback Method
cpg	489.08	J/mol×K	826.76	Joback Method
cpg	497.70	J/mol×K	859.91	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=R106362&Units=SI

Legend

cpg:	Ideal gas heat capacity
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