Oo-t-butyl o-methylsuccinate

Inchi: InChI=1S/C9H16O5/c1-9(2,3)14-13-8(11)6-5-7(10)12-4/h5-6H2,1-4H3
InchiKey: VAMBMSNSIPIASM-UHFFFAOYSA-N
Formula: C9H16O5
SMILES: COC(=O)CCC(=O)OOC(C)(C)C
Mol. weight [g/mol]: 204.22
CAS: 29269-20-3

Physical Properties

Property code	Value	Unit	Source
gf	-545.10	kJ/mol	Joback Method
hf	-859.66	kJ/mol	Joback Method
hfl	-841.00 ± 3.00	kJ/mol	NIST Webbook
hfus	18.41	kJ/mol	Joback Method
hvap	55.05	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.213		Crippen Method
mcvol	158.420	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
tb	577.09	K	Joback Method
tc	767.73	K	Joback Method
tf	360.16	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.16	J/mol×K	577.09	Joback Method
cpg	409.08	J/mol×K	608.86	Joback Method
cpg	421.41	J/mol×K	640.64	Joback Method
cpg	433.14	J/mol×K	672.41	Joback Method
cpg	444.28	J/mol×K	704.19	Joback Method
cpg	454.81	J/mol×K	735.96	Joback Method
cpg	464.73	J/mol×K	767.73	Joback Method
dvisc	0.0015949	Pa×s	360.16	Joback Method

dvisc	0.0009004	Pa×s	396.31	Joback Method
dvisc	0.0005593	Pa×s	432.47	Joback Method
dvisc	0.0003739	Pa×s	468.62	Joback Method
dvisc	0.0002648	Pa×s	504.78	Joback Method
dvisc	0.0001964	Pa×s	540.93	Joback Method
dvisc	0.0001512	Pa×s	577.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29269203&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
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume