Oo-tert-butyl o-methylperfumarate

Inchi: InChI=1S/C9H14O5/c1-9(2,3)14-13-8(11)6-5-7(10)12-4/h5-6H,1-4H3/b6-5+
InchiKey: WVSJZOKBOUVTBA-AATRIKPKSA-N
Formula: C9H14O5
SMILES: COC(=O)C=CC(=O)OOC(C)(C)C
Mol. weight [g/mol]: 202.20
CAS: 52345-49-0

Physical Properties

Property code	Value	Unit	Source
gf	-464.88	kJ/mol	Joback Method
hf	-742.44	kJ/mol	Joback Method
hfl	-747.00 ± 2.00	kJ/mol	NIST Webbook
hfus	18.62	kJ/mol	Joback Method
hvap	55.01	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	0.989		Crippen Method
mcvol	154.120	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	581.25	K	Joback Method
tc	779.77	K	Joback Method
tf	355.08	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.32	J/mol×K	581.25	Joback Method
cpg	431.99	J/mol×K	746.68	Joback Method
cpg	422.10	J/mol×K	713.60	Joback Method
cpg	411.60	J/mol×K	680.51	Joback Method
cpg	400.47	J/mol×K	647.42	Joback Method
cpg	388.72	J/mol×K	614.34	Joback Method
cpg	441.27	J/mol×K	779.77	Joback Method
dvisc	0.0001283	Pa×s	581.25	Joback Method

dvisc	0.0001674	Pa×s	543.56	Joback Method
dvisc	0.0002274	Pa×s	505.86	Joback Method
dvisc	0.0003245	Pa×s	468.17	Joback Method
dvisc	0.0004927	Pa×s	430.47	Joback Method
dvisc	0.0008106	Pa×s	392.78	Joback Method
dvisc	0.0014824	Pa×s	355.08	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=C52345490&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
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