Isopropyl tiglate

Other names:	2-Butenoic acid, 2-methyl-, 1-methylethyl ester, (E)-
	2-Butenoic acid, 2-methyl, 1-isopropyl ester (E)-
	Isopropyl 2-methyl-2-butenoate
	Isopropyl «alpha»-methyl crotonate
	Isopropyl (2E)-2-methyl-2-butenoate
	2-Butenoic acid, 2-methyl-, 1-methylethyl ester, (2E)-
	Tiglic acid isopropyl ester
	isopropyl 2-methylcrotonate
Inchi:	InChI=1S/C8H14O2/c1-5-7(4)8(9)10-6(2)3/h5-6H,1-4H3/b7-5+
InchiKey:	VUPBIVVRPJDWNW-FNORWQNLSA-N
Formula:	C8H14O2
SMILES:	CC=C(C)C(=O)OC(C)C
Mol. weight [g/mol]:	142.20
CAS:	1733-25-1

Physical Properties

Property code	Value	Unit	Source
gf	-148.21	kJ/mol	Joback Method
hf	-351.10	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	42.21	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.904		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
rinpol	952.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	952.00		NIST Webbook
ripol	1238.00		NIST Webbook
tb	462.33	K	Joback Method
tc	653.28	K	Joback Method
tf	218.04	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.35	J/mol×K	462.33	Joback Method
cpg	275.79	J/mol×K	494.15	Joback Method
cpg	287.69	J/mol×K	525.98	Joback Method
cpg	299.05	J/mol×K	557.80	Joback Method
cpg	309.90	J/mol×K	589.63	Joback Method
cpg	320.24	J/mol×K	621.45	Joback Method
cpg	330.09	J/mol×K	653.28	Joback Method

Sources

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=C1733251&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume