Isobutyric acid, tert-butyl ester

Other names: Propanoic acid, 2-methyl-, 1,1-dimethylethyl ester
Inchi: InChI=1S/C8H16O2/c1-6(2)7(9)10-8(3,4)5/h6H,1-5H3
InchiKey: KVWOTUDBCFBGFJ-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CC(C)C(=O)OC(C)(C)C
Mol. weight [g/mol]: 144.21
CAS: 16889-72-8

Physical Properties

Property code	Value	Unit	Source
gf	-217.04	kJ/mol	Joback Method
hf	-467.28	kJ/mol	Joback Method
hfus	8.33	kJ/mol	Joback Method
hvap	40.87	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.984		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	816.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	816.00		NIST Webbook
ripol	956.00		NIST Webbook
ripol	956.00		NIST Webbook
tb	455.06	K	Joback Method
tc	645.31	K	Joback Method
tf	239.50	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.43	J/mol×K	455.06	Joback Method
cpg	296.22	J/mol×K	486.77	Joback Method
cpg	309.37	J/mol×K	518.48	Joback Method

cpg	321.89	J/mol×K	550.18	Joback Method
cpg	333.80	J/mol×K	581.89	Joback Method
cpg	345.10	J/mol×K	613.60	Joback Method
cpg	355.83	J/mol×K	645.31	Joback Method
dvisc	0.0072531	Pa×s	239.50	Joback Method
dvisc	0.0028574	Pa×s	275.43	Joback Method
dvisc	0.0013957	Pa×s	311.35	Joback Method
dvisc	0.0007906	Pa×s	347.28	Joback Method
dvisc	0.0004982	Pa×s	383.21	Joback Method
dvisc	0.0003399	Pa×s	419.13	Joback Method
dvisc	0.0002462	Pa×s	455.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16889728&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume