Acetic acid, 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C8H16O2/c1-6(8(3,4)5)10-7(2)9/h6H,1-5H3
InchiKey: MAYGVGMOSXYCRX-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 144.21
CAS: 616-51-3

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	881.00		NIST Webbook
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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	345.10	J/mol×K	613.60	Joback Method
cpg	333.80	J/mol×K	581.89	Joback Method
cpg	321.89	J/mol×K	550.18	Joback Method
cpg	309.37	J/mol×K	518.48	Joback Method
cpg	296.22	J/mol×K	486.77	Joback Method
cpg	355.83	J/mol×K	645.31	Joback Method

dvisc	0.0002462	Pa×s	455.06	Joback Method
dvisc	0.0003399	Pa×s	419.13	Joback Method
dvisc	0.0004982	Pa×s	383.21	Joback Method
dvisc	0.0007906	Pa×s	347.28	Joback Method
dvisc	0.0013957	Pa×s	311.35	Joback Method
dvisc	0.0028574	Pa×s	275.43	Joback Method
dvisc	0.0072531	Pa×s	239.50	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=C616513&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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