Acetic acid, 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C10H20O2/c1-8(6-10(3,4)5)7-12-9(2)11/h8H,6-7H2,1-5H3
InchiKey: VCSSZPFJAXWTBM-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 172.26

Physical Properties

Property code	Value	Unit	Source
gf	-200.20	kJ/mol	Joback Method
hf	-508.56	kJ/mol	Joback Method
hfus	13.51	kJ/mol	Joback Method
hvap	45.33	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.622		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1082.00		NIST Webbook
tb	500.82	K	Joback Method
tc	686.98	K	Joback Method
tf	262.04	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.17	J/mol×K	500.82	Joback Method
cpg	442.02	J/mol×K	655.96	Joback Method
cpg	429.24	J/mol×K	624.93	Joback Method
cpg	415.78	J/mol×K	593.90	Joback Method
cpg	401.63	J/mol×K	562.87	Joback Method
cpg	386.77	J/mol×K	531.85	Joback Method
cpg	454.15	J/mol×K	686.98	Joback Method
dvisc	0.0002041	Pa×s	500.82	Joback Method
dvisc	0.0002831	Pa×s	461.02	Joback Method

dvisc	0.0004178	Pa×s	421.23	Joback Method
dvisc	0.0006687	Pa×s	381.43	Joback Method
dvisc	0.0011942	Pa×s	341.63	Joback Method
dvisc	0.0024849	Pa×s	301.84	Joback Method
dvisc	0.0064596	Pa×s	262.04	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368953&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume