Hexanoic acid, 3,5,5-trimethyl-

Other names: 3,5,5-Trimethylhexanoic acid
Inchi: InChI=1S/C9H18O2/c1-7(5-8(10)11)6-9(2,3)4/h7H,5-6H2,1-4H3,(H,10,11)
InchiKey: OILUAKBAMVLXGF-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CC(CC(=O)O)CC(C)(C)C
Mol. weight [g/mol]: 158.24
CAS: 3302-10-1

Physical Properties

Property code	Value	Unit	Source
gf	-240.44	kJ/mol	Joback Method
hf	-507.93	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	57.37	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.533		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1139.00		NIST Webbook
tb	547.70	K	Joback Method
tc	727.60	K	Joback Method
tf	289.36	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.91	J/mol×K	547.70	Joback Method
cpg	371.56	J/mol×K	577.68	Joback Method
cpg	383.56	J/mol×K	607.67	Joback Method
cpg	394.94	J/mol×K	637.65	Joback Method
cpg	405.72	J/mol×K	667.63	Joback Method
cpg	415.94	J/mol×K	697.62	Joback Method
cpg	425.62	J/mol×K	727.60	Joback Method

dvisc	0.0282170	Pa×s	289.36	Joback Method
dvisc	0.0061539	Pa×s	332.42	Joback Method
dvisc	0.0019031	Pa×s	375.47	Joback Method
dvisc	0.0007493	Pa×s	418.53	Joback Method
dvisc	0.0003510	Pa×s	461.59	Joback Method
dvisc	0.0001872	Pa×s	504.64	Joback Method
dvisc	0.0001102	Pa×s	547.70	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56981e+01
Coeff. B	-4.68506e+03
Coeff. C	-8.13040e+01
Temperature range (K), min.	385.32
Temperature range (K), max.	532.37

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C3302101&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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume