

3,5,5-Trimethylhexyl acetate

Other names:	1-Hexanol, 3,5,5-trimethyl-, acetate 3,5,5-Trimethyl-1-hexanol acetate Acetic acid 3,5,5-trimethylhexyl ester Isononyl acetate
Inchi:	InChI=1S/C11H22O2/c1-9(8-11(3,4)5)6-7-13-10(2)12/h9H,6-8H2,1-5H3
InchiKey:	DGKXDLCVQSQVBC-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CC(=O)OCCC(C)CC(C)(C)C
Mol. weight [g/mol]:	186.29
CAS:	58430-94-7

Physical Properties

Property code	Value	Unit	Source
gf	-191.78	kJ/mol	Joback Method
hf	-529.20	kJ/mol	Joback Method
hfus	16.10	kJ/mol	Joback Method
hvap	47.55	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.012		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1162.00		NIST Webbook
rinpol	1180.00		NIST Webbook
ripol	1430.00		NIST Webbook
tb	523.70	K	Joback Method
tc	707.84	K	Joback Method
tf	273.31	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.38	J/mol×K	523.70	Joback Method
cpg	434.70	J/mol×K	554.39	Joback Method

cpg	450.26	J/mol×K	585.08	Joback Method
cpg	465.08	J/mol×K	615.77	Joback Method
cpg	479.16	J/mol×K	646.46	Joback Method
cpg	492.55	J/mol×K	677.15	Joback Method
cpg	505.25	J/mol×K	707.84	Joback Method
dvisc	0.0059930	Pa×s	273.31	Joback Method
dvisc	0.0022813	Pa×s	315.04	Joback Method
dvisc	0.0010885	Pa×s	356.77	Joback Method
dvisc	0.0006065	Pa×s	398.50	Joback Method
dvisc	0.0003775	Pa×s	440.24	Joback Method
dvisc	0.0002551	Pa×s	481.97	Joback Method
dvisc	0.0001835	Pa×s	523.70	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35503e+01
Coeff. B	-3.77017e+03
Coeff. C	-7.18520e+01
Temperature range (K), min.	356.12
Temperature range (K), max.	529.46

Sources

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=C58430947&Units=SI
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/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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