3-Methylpentyl acetate

Inchi: InChI=1S/C8H16O2/c1-4-7(2)5-6-10-8(3)9/h7H,4-6H2,1-3H3
InchiKey: NFYJZIICTJCGOR-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCC(C)CCOC(C)=O
Mol. weight [g/mol]: 144.21
CAS: 35897-13-3

Physical Properties

Property code	Value	Unit	Source
af	0.4743		Cheméo Relay (1.0)
gf	-219.88	kJ/mol	Joback Method
hf	-547.52	kJ/mol	Cheméo Relay (1.0)
hfus	15.74	kJ/mol	Joback Method
hvap	48.53	kJ/mol	Cheméo Relay (1.0)
ie	9.79	eV	Cheméo Relay (1.0)
log10ws	-2.21		Cheméo Relay (1.0)
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	980.20		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	980.20		NIST Webbook
rinpol	993.00		NIST Webbook
tb	433.50	K	Cheméo Relay (1.0)
tc	608.85	K	Cheméo Relay (1.0)
tf	191.00	K	Cheméo Relay (1.0)
vc	0.476	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method

cpg	316.22	J/mol×K	547.72	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method
cpg	338.23	J/mol×K	607.34	Joback Method
cpg	348.57	J/mol×K	637.16	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51982e+01
Coeff. B	-3.95841e+03
Coeff. C	-6.18440e+01
Temperature range (K), min.	327.32
Temperature range (K), max.	462.22

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35897133&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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