2-Methylpentan-2-yl acetate

Inchi: InChI=1S/C8H16O2/c1-5-6-8(3,4)10-7(2)9/h5-6H2,1-4H3
InchiKey: ZBIZLXMISNHYIG-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCCC(C)(C)OC(C)=O
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
hf	-559.21	kJ/mol	Cheméo Relay (1.0)
hfus	11.85	kJ/mol	Joback Method
hvap	45.60	kJ/mol	NIST Webbook
log10ws	-1.78		Cheméo Relay (1.0)
logp	2.128		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
tb	413.39	K	Cheméo Relay (1.0)
tf	198.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.32	J/mol×K	455.50	Joback Method
cpg	295.73	J/mol×K	486.51	Joback Method
cpg	308.53	J/mol×K	517.51	Joback Method
cpg	320.73	J/mol×K	548.52	Joback Method
cpg	332.35	J/mol×K	579.53	Joback Method
cpg	343.41	J/mol×K	610.54	Joback Method
cpg	353.92	J/mol×K	641.54	Joback Method
dvisc	0.0046923	Pa×s	254.50	Joback Method
dvisc	0.0021847	Pa×s	288.00	Joback Method
dvisc	0.0011929	Pa×s	321.50	Joback Method
dvisc	0.0007301	Pa×s	355.00	Joback Method
dvisc	0.0004864	Pa×s	388.50	Joback Method
dvisc	0.0003456	Pa×s	422.00	Joback Method

dvisc	0.0002582	Pa×s	455.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	307.70	K	1.30	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C34859988&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):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.