2-Pentanol, 2-methyl-, 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
CAS: 34859-98-8

Physical Properties

Property code	Value	Unit	Source
gf	-214.60	kJ/mol	Joback Method
hf	-462.00	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	45.60	kJ/mol	NIST Webbook
log10ws	-2.15		Crippen Method
logp	2.128		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
tb	455.50	K	Joback Method
tc	641.54	K	Joback Method
tf	254.50	K	Joback Method
vc	0.496	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34859988&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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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