

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/molxK	455.50	Joback Method
cpg	343.41	J/molxK	610.54	Joback Method
cpg	332.35	J/molxK	579.53	Joback Method
cpg	320.73	J/molxK	548.52	Joback Method
cpg	308.53	J/molxK	517.51	Joback Method
cpg	295.73	J/molxK	486.51	Joback Method
cpg	353.92	J/molxK	641.54	Joback Method
dvisc	0.0002582	Paxs	455.50	Joback Method
dvisc	0.0003456	Paxs	422.00	Joback Method

dvisc	0.0004864	Paxs	388.50	Joback Method
dvisc	0.0007301	Paxs	355.00	Joback Method
dvisc	0.0011929	Paxs	321.50	Joback Method
dvisc	0.0021847	Paxs	288.00	Joback Method
dvisc	0.0046923	Paxs	254.50	Joback Method

Pressure Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C34859988&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
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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