2-Pentanol, 3-methylbutanoate

Inchi: InChI=1S/C10H20O2/c1-5-6-9(4)12-10(11)7-8(2)3/h8-9H,5-7H2,1-4H3
InchiKey: DUJBVANUBSYWGF-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CCCC(C)OC(=O)CC(C)C
Mol. weight [g/mol]: 172.26

Physical Properties

Property code	Value	Unit	Source
gf	-205.48	kJ/mol	Joback Method
hf	-505.09	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	46.23	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.764		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1059.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1059.00		NIST Webbook
tb	503.61	K	Joback Method
tc	682.96	K	Joback Method
tf	244.62	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.51	J/mol×K	503.61	Joback Method
cpg	383.39	J/mol×K	533.50	Joback Method
cpg	397.67	J/mol×K	563.39	Joback Method
cpg	411.38	J/mol×K	593.28	Joback Method
cpg	424.51	J/mol×K	623.18	Joback Method
cpg	437.08	J/mol×K	653.07	Joback Method

cpg	449.08	J/mol×K	682.96	Joback Method
dvisc	0.0070487	Pa×s	244.62	Joback Method
dvisc	0.0024917	Pa×s	287.79	Joback Method
dvisc	0.0011553	Pa×s	330.95	Joback Method
dvisc	0.0006396	Pa×s	374.12	Joback Method
dvisc	0.0004002	Pa×s	417.28	Joback Method
dvisc	0.0002734	Pa×s	460.44	Joback Method
dvisc	0.0001994	Pa×s	503.61	Joback Method

Sources

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=R75503&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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