Propyl 2-methylvalerate

Other names: Propyl 2-methylpentanoate
Inchi: InChI=1S/C9H18O2/c1-4-6-8(3)9(10)11-7-5-2/h8H,4-7H2,1-3H3
InchiKey: AJYNZTLCODJWQR-UHFFFAOYSA-N
Formula: C9H18O2
SMILES: CCCOC(=O)C(C)CCC
Mol. weight [g/mol]: 158.24
CAS: 6639-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-211.46	kJ/mol	Joback Method
hf	-479.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1009.00		NIST Webbook
rinpol	1009.00		NIST Webbook
tb	481.17	K	Joback Method
tc	658.49	K	Joback Method
tf	248.35	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	386.04	J/mol×K	628.93	Joback Method
cpg	374.44	J/mol×K	599.38	Joback Method
cpg	362.35	J/mol×K	569.83	Joback Method
cpg	349.76	J/mol×K	540.28	Joback Method
cpg	336.66	J/mol×K	510.72	Joback Method

cpg	397.15	J/mol×K	658.49	Joback Method
dvisc	0.0002272	Pa×s	481.17	Joback Method
dvisc	0.0003022	Pa×s	442.37	Joback Method
dvisc	0.0004246	Pa×s	403.56	Joback Method
dvisc	0.0006412	Pa×s	364.76	Joback Method
dvisc	0.0010682	Pa×s	325.96	Joback Method
dvisc	0.0020429	Pa×s	287.15	Joback Method
dvisc	0.0047844	Pa×s	248.35	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=C6639141&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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