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

Physical Properties

Property code	Value	Unit	Source
hf	-556.55	kJ/mol	Cheméo Relay (1.0)
hfus	18.33	kJ/mol	Joback Method
hvap	46.71	kJ/mol	Cheméo Relay (1.0)
ie	9.68	eV	Cheméo Relay (1.0)
log10ws	-2.52		Cheméo Relay (1.0)
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	428.44	K	Cheméo Relay (1.0)
tc	615.72	K	Cheméo Relay (1.0)
tf	202.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	397.15	J/mol×K	658.49	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
dvisc	0.0006412	Pa×s	364.76	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	0.0047844	Pa×s	248.35	Joback Method
dvisc	0.0010682	Pa×s	325.96	Joback Method
dvisc	0.0020429	Pa×s	287.15	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6639141&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
ie: Ionization energy
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