4-Methylpentyl isobutyrate

Inchi: InChI=1S/C10H20O2/c1-8(2)6-5-7-12-10(11)9(3)4/h8-9H,5-7H2,1-4H3
InchiKey: AJCVRKAWPQPCAA-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CC(C)CCCOC(=O)C(C)C
Mol. weight [g/mol]: 172.27

Physical Properties

Property code	Value	Unit	Source
af	0.5495		Cheméo Relay (1.0)
hf	-592.32	kJ/mol	Cheméo Relay (1.0)
hfus	17.40	kJ/mol	Joback Method
hvap	49.95	kJ/mol	Cheméo Relay (1.0)
ie	9.75	eV	Cheméo Relay (1.0)
log10ws	-2.87		Cheméo Relay (1.0)
logp	2.622		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1109.50		NIST Webbook
rinpol	1109.50		NIST Webbook
tb	449.75	K	Cheméo Relay (1.0)
tc	631.37	K	Cheméo Relay (1.0)
tf	208.01	K	Cheméo Relay (1.0)
vc	0.600	m3/kmol	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35852449&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):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
vc:	Critical Volume