

isobutyl 5-hexenoate

Inchi:	InChI=1S/C10H18O2/c1-4-5-6-7-10(11)12-8-9(2)3/h4,9H,1,5-8H2,2-3H3
InchiKey:	CQKOOZOPDPSYIW-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	C=CCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-115.20	kJ/mol	Joback Method
hf	-374.38	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.542		Crippen Method
mvol	154.900	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
ripol	1386.00		NIST Webbook
ripol	1394.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1394.00		NIST Webbook
ripol	1386.00		NIST Webbook
tb	500.73	K	Joback Method
tc	679.83	K	Joback Method
tf	257.86	K	Joback Method
vc	0.595	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.06	J/molxK	500.73	Joback Method
cpg	414.23	J/molxK	649.98	Joback Method
cpg	402.50	J/molxK	620.13	Joback Method
cpg	390.22	J/molxK	590.28	Joback Method
cpg	377.40	J/molxK	560.43	Joback Method

cpg	364.01	J/mol×K	530.58	Joback Method
cpg	425.43	J/mol×K	679.83	Joback Method
dvisc	0.0002145	Paxs	500.73	Joback Method
dvisc	0.0002837	Paxs	460.25	Joback Method
dvisc	0.0003961	Paxs	419.77	Joback Method
dvisc	0.0005939	Paxs	379.29	Joback Method
dvisc	0.0009808	Paxs	338.82	Joback Method
dvisc	0.0018562	Paxs	298.34	Joback Method
dvisc	0.0042919	Paxs	257.86	Joback Method

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=R313689&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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