Hexanoic acid, 2-ethyl-, 2-methylpropyl ester

Other names: Isobutyl 2-ethylhexanoate
iso-Butyl 2-ethyl n-hexanoate
Inchi: InChI=1S/C12H24O2/c1-5-7-8-11(6-2)12(13)14-9-10(3)4/h10-11H,5-9H2,1-4H3
InchiKey: FPBZIVPZCGICNQ-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CCCCC(CC)C(=O)OCC(C)C
Mol. weight [g/mol]: 200.32
CAS: 7434-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-188.64	kJ/mol	Joback Method
hf	-546.37	kJ/mol	Joback Method
hfus	22.58	kJ/mol	Joback Method
hvap	50.69	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.402		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	1248.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook
tb	549.37	K	Joback Method
tc	725.46	K	Joback Method
tf	267.16	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.71	J/mol×K	549.37	Joback Method
cpg	481.08	J/mol×K	578.72	Joback Method
cpg	496.78	J/mol×K	608.07	Joback Method
cpg	511.82	J/mol×K	637.42	Joback Method

cpg	526.20	J/mol×K	666.76	Joback Method
cpg	539.94	J/mol×K	696.11	Joback Method
cpg	553.06	J/mol×K	725.46	Joback Method
dvisc	0.0062070	Pa×s	267.16	Joback Method
dvisc	0.0021594	Pa×s	314.19	Joback Method
dvisc	0.0009890	Pa×s	361.23	Joback Method
dvisc	0.0005423	Pa×s	408.26	Joback Method
dvisc	0.0003366	Pa×s	455.30	Joback Method
dvisc	0.0002285	Pa×s	502.33	Joback Method
dvisc	0.0001657	Pa×s	549.37	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7434891&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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