

2-Ethylbutyric acid, 3-methylpent-2-yl ester

Inchi:	InChI=1S/C12H24O2/c1-6-9(4)10(5)14-12(13)11(7-2)8-3/h9-11H,6-8H2,1-5H3
InchiKey:	FIFBFJZXKMNFX-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCC(CC)C(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	200.32

Physical Properties

Property code	Value	Unit	Source
gf	-191.08	kJ/mol	Joback Method
hf	-551.65	kJ/mol	Joback Method
hfus	19.05	kJ/mol	Joback Method
hvap	50.30	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.400		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinqol	1176.00		NIST Webbook
tb	548.93	K	Joback Method
tc	728.36	K	Joback Method
tf	252.16	K	Joback Method
vc	0.714	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.98	J/molxK	548.93	Joback Method
cpg	541.73	J/molxK	698.45	Joback Method
cpg	527.75	J/molxK	668.55	Joback Method
cpg	513.09	J/molxK	638.64	Joback Method
cpg	497.75	J/molxK	608.74	Joback Method
cpg	481.72	J/molxK	578.83	Joback Method
cpg	555.06	J/molxK	728.36	Joback Method
dvisc	0.0001557	Paxs	548.93	Joback Method
dvisc	0.0002202	Paxs	499.47	Joback Method

dvisc	0.0003362	Paxs	450.01	Joback Method
dvisc	0.0005697	Paxs	400.54	Joback Method
dvisc	0.0011201	Paxs	351.08	Joback Method
dvisc	0.0027490	Paxs	301.62	Joback Method
dvisc	0.0095948	Paxs	252.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369746&Units=SI
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

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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