

2-Ethylbutyric acid, tetrahydrofurfuryl ester

Inchi:	InChI=1S/C11H20O3/c1-3-9(4-2)11(12)14-8-10-6-5-7-13-10/h9-10H,3-8H2,1-2H3
InchiKey:	XDCJLVSQPWWLJL-UHFFFAOYSA-N
Formula:	C11H20O3
SMILES:	CCC(CC)C(=O)OCC1CCCO1
Mol. weight [g/mol]:	200.27

Physical Properties

Property code	Value	Unit	Source
gf	-244.19	kJ/mol	Joback Method
hf	-591.97	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	53.61	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.145		Crippen Method
mcvol	168.300	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1355.00		NIST Webbook
rinpol	1355.00		NIST Webbook
tb	569.16	K	Joback Method
tc	767.57	K	Joback Method
tf	308.36	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.52	J/molxK	569.16	Joback Method
cpg	453.82	J/molxK	602.23	Joback Method
cpg	470.23	J/molxK	635.30	Joback Method
cpg	485.77	J/molxK	668.36	Joback Method
cpg	500.46	J/molxK	701.43	Joback Method
cpg	514.32	J/molxK	734.50	Joback Method
cpg	527.36	J/molxK	767.57	Joback Method
dvisc	0.0042840	Paxs	308.36	Joback Method

dvisc	0.0020090	Paxs	351.83	Joback Method
dvisc	0.0011128	Paxs	395.29	Joback Method
dvisc	0.0006930	Paxs	438.76	Joback Method
dvisc	0.0004700	Paxs	482.23	Joback Method
dvisc	0.0003399	Paxs	525.69	Joback Method
dvisc	0.0002583	Paxs	569.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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