

(E)-3-methyl-2-pentenoic acid

Inchi:	InChI=1S/C6H10O2/c1-3-4-5(2)6(7)8/h3-5H,1-2H3,(H,7,8)/b4-3+
InchiKey:	NFRJJFMXYKSRPK-ONEGZZNKSA-N
Formula:	C6H10O2
SMILES:	CC=CC(C)C(=O)O
Mol. weight [g/mol]:	114.14

Physical Properties

Property code	Value	Unit	Source
gf	-188.32	kJ/mol	Joback Method
hf	-320.04	kJ/mol	Joback Method
hfus	13.66	kJ/mol	Joback Method
hvap	51.94	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.283		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
ripol	1892.00		NIST Webbook
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tb	486.45	K	Joback Method
tc	669.30	K	Joback Method
tf	248.05	K	Joback Method
vc	0.370	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.34	J/molxK	486.45	Joback Method
cpg	215.01	J/molxK	516.92	Joback Method
cpg	223.25	J/molxK	547.40	Joback Method
cpg	231.07	J/molxK	577.87	Joback Method
cpg	238.49	J/molxK	608.35	Joback Method
cpg	245.53	J/molxK	638.82	Joback Method
cpg	252.21	J/molxK	669.30	Joback Method
dvisc	0.0452390	Paxs	248.05	Joback Method

dvisc	0.0092323	Paxs	287.78	Joback Method
dvisc	0.0027706	Paxs	327.52	Joback Method
dvisc	0.0010788	Paxs	367.25	Joback Method
dvisc	0.0005050	Paxs	406.98	Joback Method
dvisc	0.0002706	Paxs	446.72	Joback Method
dvisc	0.0001605	Paxs	486.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R335045&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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