

3-Ethyl-3-methyl-2-pentanol

Inchi:	InChI=1S/C8H18O/c1-5-8(4,6-2)7(3)9/h7,9H,5-6H2,1-4H3
InchiKey:	SLBLSROGXMXPFF-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CCC(C)(CC)C(C)O
Mol. weight [g/mol]:	130.23
CAS:	66576-22-5

Physical Properties

Property code	Value	Unit	Source
gf	-119.94	kJ/mol	Joback Method
hf	-374.71	kJ/mol	Joback Method
hfus	9.63	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
ripol	1386.00		NIST Webbook
tb	470.95	K	Joback Method
tc	643.32	K	Joback Method
tf	228.16	K	Joback Method
vc	0.485	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.99	J/molxK	470.95	Joback Method
cpg	305.85	J/molxK	499.68	Joback Method
cpg	318.10	J/molxK	528.41	Joback Method
cpg	329.77	J/molxK	557.13	Joback Method
cpg	340.87	J/molxK	585.86	Joback Method
cpg	351.43	J/molxK	614.59	Joback Method
cpg	361.48	J/molxK	643.32	Joback Method
dvisc	0.1736472	Paxs	228.16	Joback Method

dvisc	0.0230030	Paxs	268.62	Joback Method
dvisc	0.0051732	Paxs	309.09	Joback Method
dvisc	0.0016435	Paxs	349.55	Joback Method
dvisc	0.0006624	Paxs	390.02	Joback Method
dvisc	0.0003167	Paxs	430.49	Joback Method
dvisc	0.0001719	Paxs	470.95	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=C66576225&Units=SI

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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