

2-Propanol, 1-chloro-3-(1-methylethoxy)-

Other names:	2-Propanol, 1-chloro-3-isopropoxy- 1-Chloro-3-isopropoxy-2-propanol 1-Chloro-3-(pentyloxy)-2-propanol U 25,352 1-chloro-3-isopropoxypropan-2-ol
Inchi:	InChI=1S/C6H13ClO2/c1-5(2)9-4-6(8)3-7/h5-6,8H,3-4H2,1-2H3
InchiKey:	GQPJSBQMFFGZAU-UHFFFAOYSA-N
Formula:	C6H13ClO2
SMILES:	CC(C)OCC(O)CCl
Mol. weight [g/mol]:	152.62
CAS:	4288-84-0

Physical Properties

Property code	Value	Unit	Source
gf	-258.99	kJ/mol	Joback Method
hf	-477.92	kJ/mol	Joback Method
hfus	13.72	kJ/mol	Joback Method
hvap	51.65	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.011		Crippen Method
mcvol	119.380	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
tb	487.83	K	Joback Method
tc	661.81	K	Joback Method
tf	240.35	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.00	J/molxK	487.83	Joback Method
cpg	265.60	J/molxK	516.83	Joback Method

cpg	274.83	J/molxK	545.82	Joback Method
cpg	283.71	J/molxK	574.82	Joback Method
cpg	292.24	J/molxK	603.82	Joback Method
cpg	300.42	J/molxK	632.81	Joback Method
cpg	308.26	J/molxK	661.81	Joback Method
dvisc	0.0772383	Paxs	240.35	Joback Method
dvisc	0.0126866	Paxs	281.60	Joback Method
dvisc	0.0033061	Paxs	322.84	Joback Method
dvisc	0.0011684	Paxs	364.09	Joback Method
dvisc	0.0005103	Paxs	405.34	Joback Method
dvisc	0.0002597	Paxs	446.58	Joback Method
dvisc	0.0001482	Paxs	487.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4288840&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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