

1-Phenoxypropan-2-ol

Other names:	Phenyl-«beta»-hydroxypropyl ether 1-Phenoxy-2-propanol 2-Propanol, 1-phenoxy- Phenoxyisopropanol Propylene phenoxetol 2-Phenoxy-1-methylethanol Propylenephenoxythol Propylene glycol 1-phenyl ether
Inchi:	InChI=1S/C9H12O2/c1-8(10)7-11-9-5-3-2-4-6-9/h2-6,8,10H,7H2,1H3
InchiKey:	IBLKWZIFZMJLFL-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CC(O)COc1ccccc1
Mol. weight [g/mol]:	152.19
CAS:	770-35-4

Physical Properties

Property code	Value	Unit	Source
gf	-106.95	kJ/mol	Joback Method
hf	-282.29	kJ/mol	Joback Method
hfus	14.86	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.446		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	1246.40		NIST Webbook
rinpol	1214.80		NIST Webbook
rinpol	1214.80		NIST Webbook
tb	546.16	K	Joback Method
tc	743.59	K	Joback Method
tf	285.66	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.72	J/molxK	743.59	Joback Method
cpg	342.94	J/molxK	710.68	Joback Method
cpg	333.61	J/molxK	677.78	Joback Method
cpg	323.69	J/molxK	644.87	Joback Method
cpg	313.19	J/molxK	611.97	Joback Method
cpg	302.08	J/molxK	579.06	Joback Method
cpg	290.35	J/molxK	546.16	Joback Method
dvisc	0.0150105	Paxs	285.66	Joback Method
dvisc	0.0000890	Paxs	546.16	Joback Method
dvisc	0.0001447	Paxs	502.74	Joback Method
dvisc	0.0002578	Paxs	459.33	Joback Method
dvisc	0.0005180	Paxs	415.91	Joback Method
dvisc	0.0012248	Paxs	372.49	Joback Method
dvisc	0.0036345	Paxs	329.08	Joback Method
hvapt	59.50	kJ/mol	449.00	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C770354&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

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
hvapt:	Enthalpy of vaporization at a given temperature

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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