

1-Propanol, 3-phenoxy-

Other names:	3-Phenoxy-1-propanol 3-phenoxypropan-1-ol
Inchi:	InChI=1S/C9H12O2/c10-7-4-8-11-9-5-2-1-3-6-9/h1-3,5-6,10H,4,7-8H2
InchiKey:	AWVDYRFLCAZENH-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	OCCCOc1ccccc1
Mol. weight [g/mol]:	152.19
CAS:	6180-61-6

Physical Properties

Property code	Value	Unit	Source
gf	-104.51	kJ/mol	Joback Method
hf	-277.01	kJ/mol	Joback Method
hfus	18.38	kJ/mol	Joback Method
hvap	56.99	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.448		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpwl	1371.00		NIST Webbook
ripwl	2063.00		NIST Webbook
tb	546.60	K	Joback Method
tc	740.02	K	Joback Method
tf	300.66	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.99	J/mol×K	546.60	Joback Method
cpg	341.42	J/mol×K	707.78	Joback Method
cpg	332.25	J/mol×K	675.55	Joback Method
cpg	322.54	J/mol×K	643.31	Joback Method
cpg	312.27	J/mol×K	611.07	Joback Method

cpg	301.43	J/molxK	578.84	Joback Method
cpg	350.05	J/molxK	740.02	Joback Method
dvisc	0.0000946	Paxs	546.60	Joback Method
dvisc	0.0001483	Paxs	505.61	Joback Method
dvisc	0.0002518	Paxs	464.62	Joback Method
dvisc	0.0004735	Paxs	423.63	Joback Method
dvisc	0.0010196	Paxs	382.64	Joback Method
dvisc	0.0026389	Paxs	341.65	Joback Method
dvisc	0.0088520	Paxs	300.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6180616&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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