

(3-Methoxyphenyl) methanol, n-propyl

Inchi:	InChI=1S/C11H16O2/c1-3-7-13-9-10-5-4-6-11(8-10)12-2/h4-6,8H,3,7,9H2,1-2H3
InchiKey:	SWQRNWLUE NXRGB-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	CCCOCC1CCCC(OC)C1
Mol. weight [g/mol]:	180.24

Physical Properties

Property code	Value	Unit	Source
gf	-65.48	kJ/mol	Joback Method
hf	-309.75	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	47.84	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.622		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
tb	527.58	K	Joback Method
tc	727.46	K	Joback Method
tf	297.13	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.33	J/mol×K	527.58	Joback Method
cpg	366.28	J/mol×K	560.89	Joback Method
cpg	380.57	J/mol×K	594.21	Joback Method
cpg	394.19	J/mol×K	627.52	Joback Method
cpg	407.16	J/mol×K	660.83	Joback Method
cpg	419.47	J/mol×K	694.14	Joback Method
cpg	431.13	J/mol×K	727.46	Joback Method
dvisc	0.0014941	Pa×s	297.13	Joback Method

dvisc	0.0008152	Pa×s	335.54	Joback Method
dvisc	0.0005038	Pa×s	373.95	Joback Method
dvisc	0.0003405	Pa×s	412.35	Joback Method
dvisc	0.0002460	Pa×s	450.76	Joback Method
dvisc	0.0001871	Pa×s	489.17	Joback Method
dvisc	0.0001480	Pa×s	527.58	Joback Method

Sources

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=U374591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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