Benzene, (phenoxymethyl)-

Other names:	Ether, benzyl phenyl Anisole, «alpha»-phenyl- Benzyl phenyl ether Phenyl benzyl ether «alpha»-Phenylanisole Benzyloxybenzene (Phenoxymethyl)-benzene NSC 77971
Inchi:	InChI=1S/C13H12O/c1-3-7-12(8-4-1)11-14-13-9-5-2-6-10-13/h1-10H,11H2
InchiKey:	BOTNYLSAWDQNEX-UHFFFAOYSA-N
Formula:	C13H12O
SMILES:	c1ccc(COc2ccccc2)cc1
Mol. weight [g/mol]:	184.23
CAS:	946-80-5

Physical Properties

Property code	Value	Unit	Source
gf	178.40	kJ/mol	Joback Method
hf	29.19	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	51.49	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.31	eV	NIST Webbook
log10ws	-3.70		Crippen Method
logp	3.266		Crippen Method
mcvol	152.380	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
ripol	2329.00		NIST Webbook
ripol	2329.00		NIST Webbook
tb	559.70	K	NIST Webbook
tb	558.00 ± 5.00	K	NIST Webbook
tb	559.50 ± 0.50	K	NIST Webbook
tc	813.64	K	Joback Method
tf	313.00 ± 3.00	K	NIST Webbook
tf	313.00	K	NIST Webbook
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.66	J/mol×K	572.62	Joback Method
cpg	366.23	J/mol×K	612.79	Joback Method
cpg	381.58	J/mol×K	652.96	Joback Method
cpg	395.77	J/mol×K	693.13	Joback Method
cpg	408.85	J/mol×K	733.30	Joback Method
cpg	420.87	J/mol×K	773.47	Joback Method
cpg	431.89	J/mol×K	813.64	Joback Method
dvisc	0.0019671	Pa×s	311.34	Joback Method
dvisc	0.0009973	Pa×s	354.89	Joback Method
dvisc	0.0005866	Pa×s	398.43	Joback Method
dvisc	0.0003830	Pa×s	441.98	Joback Method
dvisc	0.0002700	Pa×s	485.53	Joback Method
dvisc	0.0002016	Pa×s	529.07	Joback Method
dvisc	0.0001574	Pa×s	572.62	Joback Method
hvapt	58.80	kJ/mol	464.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.00 ± 1.00	K	0.10	NIST Webbook
tbrp	397.50 ± 0.50	K	0.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C946805&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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume