Benzyl isopentyl ether

Other names:	Benzyl isoamyl ether
	Benzene, [(3-methylbutoxy)methyl]-
	Ether, benzyl isopentyl
	Isoamyl benzyl ether
	NSC 9294
	Isoamylbenzyl ester
Inchi:	InChI=1S/C12H18O/c1-11(2)8-9-13-10-12-6-4-3-5-7-12/h3-7,11H,8-10H2,1-2H3
InchiKey:	RXXCIBALSKQCAE-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CC(C)CCOCc1ccccc1
Mol. weight [g/mol]:	178.27
CAS:	122-73-6

Physical Properties

Property code	Value	Unit	Source
gf	55.13	kJ/mol	Joback Method
hf	-191.98	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	46.60	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.249		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	1310.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1309.00		NIST Webbook
ripol	1668.00		NIST Webbook
tb	522.62	K	Joback Method
tc	724.59	K	Joback Method
tf	258.65	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.16	J/mol×K	522.62	Joback Method
cpg	389.01	J/mol×K	556.28	Joback Method
cpg	404.99	J/mol×K	589.94	Joback Method
cpg	420.13	J/mol×K	623.60	Joback Method
cpg	434.45	J/mol×K	657.27	Joback Method
cpg	447.97	J/mol×K	690.93	Joback Method
cpg	460.72	J/mol×K	724.59	Joback Method
dvisc	0.0039484	Pa×s	258.65	Joback Method
dvisc	0.0015764	Pa×s	302.64	Joback Method
dvisc	0.0007945	Pa×s	346.64	Joback Method
dvisc	0.0004673	Pa×s	390.63	Joback Method
dvisc	0.0003060	Pa×s	434.63	Joback Method
dvisc	0.0002166	Pa×s	478.62	Joback Method
dvisc	0.0001625	Pa×s	522.62	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C122736&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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