Isoamyl phenylethyl ether

Other names: isopentyl phenethyl ether
Inchi: InChI=1S/C13H20O/c1-12(2)8-10-14-11-9-13-6-4-3-5-7-13/h3-7,12H,8-11H2,1-2H3
InchiKey: BHQBQWOZHYUVTL-UHFFFAOYSA-N
Formula: C13H20O
SMILES: CC(C)CCOCCc1ccccc1
Mol. weight [g/mol]: 192.30
CAS: 56011-02-0

Physical Properties

Property code	Value	Unit	Source
gf	63.55	kJ/mol	Joback Method
hf	-212.62	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	48.83	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.292		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1382.80		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1382.80		NIST Webbook
rinpol	1384.00		NIST Webbook
ripol	1741.00		NIST Webbook
ripol	1741.00		NIST Webbook
tb	545.50	K	Joback Method
tc	744.62	K	Joback Method
tf	269.92	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.36	J/mol×K	545.50	Joback Method
cpg	437.90	J/mol×K	578.69	Joback Method

cpg	454.53	J/mol×K	611.87	Joback Method
cpg	470.28	J/mol×K	645.06	Joback Method
cpg	485.18	J/mol×K	678.25	Joback Method
cpg	499.26	J/mol×K	711.43	Joback Method
cpg	512.53	J/mol×K	744.62	Joback Method
dvisc	0.0038006	Pa×s	269.92	Joback Method
dvisc	0.0014983	Pa×s	315.85	Joback Method
dvisc	0.0007481	Pa×s	361.78	Joback Method
dvisc	0.0004368	Pa×s	407.71	Joback Method
dvisc	0.0002844	Pa×s	453.64	Joback Method
dvisc	0.0002004	Pa×s	499.57	Joback Method
dvisc	0.0001498	Pa×s	545.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56011020&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
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