2-Phenethyl phenyl ether

Other names: 2-Phenylethyl phenyl ether
Inchi: InChI=1S/C14H14O/c1-3-7-13(8-4-1)11-12-15-14-9-5-2-6-10-14/h1-10H,11-12H2
InchiKey: JKSGBCQEHZWHHL-UHFFFAOYSA-N
Formula: C14H14O
SMILES: c1ccc(CCOc2ccccc2)cc1
Mol. weight [g/mol]: 198.26
CAS: 40515-89-7

Physical Properties

Property code	Value	Unit	Source
gf	186.82	kJ/mol	Joback Method
hf	8.55	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	53.72	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.308		Crippen Method
mcvol	166.470	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	595.50	K	Joback Method
tc	831.56	K	Joback Method
tf	322.61	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.13	J/mol×K	595.50	Joback Method
cpg	415.33	J/mol×K	634.84	Joback Method
cpg	431.28	J/mol×K	674.19	Joback Method
cpg	446.05	J/mol×K	713.53	Joback Method
cpg	459.69	J/mol×K	752.87	Joback Method
cpg	472.26	J/mol×K	792.21	Joback Method
cpg	483.81	J/mol×K	831.56	Joback Method
dvisc	0.0019145	Pa×s	322.61	Joback Method

dvisc	0.0009544	Pa×s	368.09	Joback Method
dvisc	0.0005545	Pa×s	413.57	Joback Method
dvisc	0.0003587	Pa×s	459.06	Joback Method
dvisc	0.0002510	Pa×s	504.54	Joback Method
dvisc	0.0001864	Pa×s	550.02	Joback Method
dvisc	0.0001448	Pa×s	595.50	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	438.00 ± 1.00	K	1.90	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40515897&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume