Benzeneethanol, «alpha»-(phenylmethyl)-

Inchi: InChI=1S/C15H16O/c16-15(11-13-7-3-1-4-8-13)12-14-9-5-2-6-10-14/h1-10,15-16H,11-12
InchiKey: CDLPUTDLLBHWRA-UHFFFAOYSA-N
Formula: C15H16O
SMILES: OC(Cc1ccccc1)Cc1ccccc1
Mol. weight [g/mol]: 212.29
CAS: 5381-92-0

Physical Properties

Property code	Value	Unit	Source
gf	160.98	kJ/mol	Joback Method
hf	-37.38	kJ/mol	Joback Method
hfus	23.25	kJ/mol	Joback Method
hvap	69.83	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.833		Crippen Method
mcvol	180.560	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	687.70	K	Joback Method
tc	907.90	K	Joback Method
tf	357.47	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.52	J/mol×K	687.70	Joback Method
cpg	543.47	J/mol×K	871.20	Joback Method
cpg	532.73	J/mol×K	834.50	Joback Method
cpg	521.13	J/mol×K	797.80	Joback Method
cpg	508.61	J/mol×K	761.10	Joback Method
cpg	495.10	J/mol×K	724.40	Joback Method
cpg	553.42	J/mol×K	907.90	Joback Method
dvisc	0.0000391	Pa×s	687.70	Joback Method
dvisc	0.0000612	Pa×s	632.66	Joback Method

dvisc	0.0001044	Pa×s	577.62	Joback Method
dvisc	0.0001993	Pa×s	522.59	Joback Method
dvisc	0.0004432	Pa×s	467.55	Joback Method
dvisc	0.0012196	Pa×s	412.51	Joback Method
dvisc	0.0045836	Pa×s	357.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	471.20	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5381920&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

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