Benzenebutanol, «alpha»-phenyl-

Inchi: InChI=1S/C16H18O/c17-16(15-11-5-2-6-12-15)13-7-10-14-8-3-1-4-9-14/h1-6,8-9,11-12,1
InchiKey: CAGIBUJGQRHYEW-UHFFFAOYSA-N
Formula: C16H18O
SMILES: OC(CCCc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 226.31
CAS: 30078-89-8

Physical Properties

Property code	Value	Unit	Source
gf	169.40	kJ/mol	Joback Method
hf	-58.02	kJ/mol	Joback Method
hfus	25.84	kJ/mol	Joback Method
hvap	72.05	kJ/mol	Joback Method
ie	8.50 ± 0.10	eV	NIST Webbook
log10ws	-4.45		Crippen Method
logp	3.743		Crippen Method
mcvol	194.650	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
tb	710.58	K	Joback Method
tc	927.27	K	Joback Method
tf	368.74	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.14	J/mol×K	710.58	Joback Method
cpg	548.08	J/mol×K	746.69	Joback Method
cpg	561.97	J/mol×K	782.81	Joback Method
cpg	574.86	J/mol×K	818.92	Joback Method
cpg	586.83	J/mol×K	855.04	Joback Method
cpg	597.94	J/mol×K	891.15	Joback Method
cpg	608.27	J/mol×K	927.27	Joback Method
dvisc	0.0038173	Pa×s	368.74	Joback Method

dvisc	0.0010182	Pa×s	425.71	Joback Method
dvisc	0.0003710	Pa×s	482.69	Joback Method
dvisc	0.0001673	Pa×s	539.66	Joback Method
dvisc	0.0000878	Pa×s	596.63	Joback Method
dvisc	0.0000516	Pa×s	653.61	Joback Method
dvisc	0.0000330	Pa×s	710.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30078898&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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume