Benzeneacetic acid, phenylmethyl ester

Other names:	Acetic acid, phenyl-, benzyl ester
	Benzyl «alpha»-toluate
	Benzyl benzeneacetate
	Benzyl phenylacetate
	Phenylacetic acid, benzyl ester
	Benzylphenylacetate fcc
Inchi:	InChI=1S/C15H14O2/c16-15(11-13-7-3-1-4-8-13)17-12-14-9-5-2-6-10-14/h1-10H,11-12H
InchiKey:	MIYFJEKZLFWKLZ-UHFFFAOYSA-N
Formula:	C15H14O2
SMILES:	O=C(Cc1ccccc1)OCc1ccccc1
Mol. weight [g/mol]:	226.27
CAS:	102-16-9

Physical Properties

Property code	Value	Unit	Source
gf	66.32	kJ/mol	Joback Method
hf	-124.67	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	62.69	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.972		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1772.40		NIST Webbook
ripol	2643.00		NIST Webbook
tb	672.25	K	Joback Method
tc	909.92	K	Joback Method
tf	383.81	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.75	J/mol×K	672.25	Joback Method
cpg	482.53	J/mol×K	711.86	Joback Method
cpg	497.08	J/mol×K	751.47	Joback Method
cpg	510.44	J/mol×K	791.09	Joback Method
cpg	522.68	J/mol×K	830.70	Joback Method
cpg	533.85	J/mol×K	870.31	Joback Method
cpg	544.01	J/mol×K	909.92	Joback Method
dvisc	0.0015219	Pa×s	383.81	Joback Method
dvisc	0.0008139	Pa×s	431.88	Joback Method
dvisc	0.0004934	Pa×s	479.96	Joback Method
dvisc	0.0003277	Pa×s	528.03	Joback Method
dvisc	0.0002330	Pa×s	576.10	Joback Method
dvisc	0.0001746	Pa×s	624.18	Joback Method
dvisc	0.0001364	Pa×s	672.25	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C102169&Units=SI

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