4-Benzyloxyphenylacetic acid

Other names: 4-(Phenylmethoxy)benzeneacetic acid
Benzeneacetic acid, 4-(phenylmethoxy)-
Inchi: InChI=1S/C15H14O3/c16-15(17)10-12-6-8-14(9-7-12)18-11-13-4-2-1-3-5-13/h1-9H,10-11
InchiKey: XJHGAJLIKDAOPE-UHFFFAOYSA-N
Formula: C15H14O3
SMILES: O=C(O)Cc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 242.27

Physical Properties

Property code	Value	Unit	Source
hf	-354.85	kJ/mol	Cheméo Relay (1.0)
hfus	29.17	kJ/mol	Joback Method
hvap	107.12	kJ/mol	Cheméo Relay (1.0)
ie	8.10	eV	Cheméo Relay (1.0)
log10ws	-3.30		Cheméo Relay (1.0)
logp	2.893		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
tb	636.75	K	Cheméo Relay (1.0)
tf	396.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.31	J/mol×K	990.02	Joback Method
cpg	560.97	J/mol×K	916.48	Joback Method
cpg	518.05	J/mol×K	769.41	Joback Method
cpg	530.17	J/mol×K	806.18	Joback Method
cpg	541.33	J/mol×K	842.95	Joback Method
cpg	551.58	J/mol×K	879.72	Joback Method
cpg	569.53	J/mol×K	953.25	Joback Method
dvisc	0.0008128	Pa×s	457.15	Joback Method
dvisc	0.0003455	Pa×s	509.19	Joback Method
dvisc	0.0001721	Pa×s	561.24	Joback Method

dvisc	0.0000965	Pa×s	613.28	Joback Method
dvisc	0.0000592	Pa×s	665.32	Joback Method
dvisc	0.0000390	Pa×s	717.37	Joback Method
dvisc	0.0000272	Pa×s	769.41	Joback Method
hfust	29.30	kJ/mol	396.10	NIST Webbook
hsubt	107.30 ± 3.00	kJ/mol	382.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6547531&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
tf:	Normal melting (fusion) point

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