4-Benzyloxypropiophenone

Other names: 4'-Benzyloxypropiophenone
4-Benzyloxypropiophenone
Propiophenone, 4'-(benzyloxy)-
p-Benzyloxypropiophenone
Inchi: InChI=1S/C16H16O2/c1-2-16(17)14-8-10-15(11-9-14)18-12-13-6-4-3-5-7-13/h3-11H,2,12
InchiKey: IKFGSOJYHVTNDV-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: CCC(=O)c1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
hfus	27.68	kJ/mol	Joback Method
hvap	89.32	kJ/mol	Cheméo Relay (1.0)
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-4.32		Cheméo Relay (1.0)
logp	3.858		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
tb	619.86	K	Cheméo Relay (1.0)
tf	353.27	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.98	J/mol×K	700.11	Joback Method
cpg	533.95	J/mol×K	739.07	Joback Method
cpg	548.72	J/mol×K	778.04	Joback Method
cpg	562.33	J/mol×K	817.00	Joback Method
cpg	574.82	J/mol×K	855.96	Joback Method
cpg	586.26	J/mol×K	894.92	Joback Method
cpg	596.69	J/mol×K	933.89	Joback Method
dvisc	0.0011644	Pa×s	407.60	Joback Method
dvisc	0.0006540	Pa×s	456.35	Joback Method
dvisc	0.0004106	Pa×s	505.10	Joback Method

dvisc	0.0002798	Pa×s	553.86	Joback Method
dvisc	0.0002029	Pa×s	602.61	Joback Method
dvisc	0.0001544	Pa×s	651.36	Joback Method
dvisc	0.0001220	Pa×s	700.11	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4495663&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point