4-Acetylbibenzyl

Other names: 1-[4-(2-phenylethyl)phenyl]ethan-1-one
Inchi: InChI=1S/C16H16O/c1-13(17)16-11-9-15(10-12-16)8-7-14-5-3-2-4-6-14/h2-6,9-12H,7-8H
InchiKey: KIRXEYNVGWVPRO-UHFFFAOYSA-N
Formula: C16H16O
SMILES: CC(=O)c1ccc(CCc2ccccc2)cc1
Mol. weight [g/mol]: 224.30

Physical Properties

Property code	Value	Unit	Source
af	0.5940		Cheméo Relay (1.0)
gf	170.11	kJ/mol	Joback Method
hf	-28.09	kJ/mol	Cheméo Relay (1.0)
hfus	26.49	kJ/mol	Joback Method
hvap	98.05	kJ/mol	Cheméo Relay (1.0)
ie	8.86	eV	Cheméo Relay (1.0)
log10ws	-4.37		Cheméo Relay (1.0)
logp	3.674		Crippen Method
mcvol	190.350	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
tb	617.31	K	Cheméo Relay (1.0)
tc	862.10	K	Cheméo Relay (1.0)
tf	338.03	K	Cheméo Relay (1.0)
vc	0.709	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.62	J/mol×K	677.69	Joback Method
cpg	573.12	J/mol×K	914.95	Joback Method
cpg	562.18	J/mol×K	875.41	Joback Method
cpg	550.29	J/mol×K	835.86	Joback Method
cpg	537.36	J/mol×K	796.32	Joback Method
cpg	523.32	J/mol×K	756.78	Joback Method
cpg	508.10	J/mol×K	717.23	Joback Method

dvisc	0.0003608	Pa×s	531.53	Joback Method
dvisc	0.0001552	Pa×s	677.69	Joback Method
dvisc	0.0001969	Pa×s	628.97	Joback Method
dvisc	0.0002598	Pa×s	580.25	Joback Method
dvisc	0.0015904	Pa×s	385.37	Joback Method
dvisc	0.0005354	Pa×s	482.81	Joback Method
dvisc	0.0008681	Pa×s	434.09	Joback Method

Sources

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=C785784&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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

Latest version available from: