1,2-Benzenedicarboxylic acid, mono(phenylmethyl) ester

Other names: Benzene-1,2-dicarboxylic acid, mono(phenylmethyl) ester
Benzene-1,2-dicarboxylic acid, monobenzyl ester
benzyl hydrogen phthalate

Inchi: InChI=1S/C15H12O4/c16-14(17)12-8-4-5-9-13(12)15(18)19-10-11-6-2-1-3-7-11/h1-9H,10

InchiKey: XIKIUQUXDNHBFR-UHFFFAOYSA-N

Formula: C15H12O4

SMILES: O=C(O)c1ccccc1C(=O)OCc1ccccc1

Mol. weight [g/mol]: 256.25

CAS: 2528-16-7

Physical Properties

Property code	Value	Unit	Source
gf	-209.05	kJ/mol	Joback Method
hf	-400.95	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	86.78	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.742		Crippen Method
mcvol	189.570	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	823.28	K	Joback Method
tc	1049.56	K	Joback Method
tf	507.08	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.41	J/mol×K	823.28	Joback Method
cpg	537.81	J/mol×K	860.99	Joback Method
cpg	547.27	J/mol×K	898.71	Joback Method
cpg	555.82	J/mol×K	936.42	Joback Method
cpg	563.51	J/mol×K	974.13	Joback Method
cpg	570.38	J/mol×K	1011.85	Joback Method

cpg	576.47	J/mol×K	1049.56	Joback Method
dvisc	0.0005269	Pa×s	507.08	Joback Method
dvisc	0.0002474	Pa×s	559.78	Joback Method
dvisc	0.0001323	Pa×s	612.48	Joback Method
dvisc	0.0000781	Pa×s	665.18	Joback Method
dvisc	0.0000498	Pa×s	717.88	Joback Method
dvisc	0.0000338	Pa×s	770.58	Joback Method
dvisc	0.0000241	Pa×s	823.28	Joback Method

Sources

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=C2528167&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume