2-Methylbenzyl benzoate

Other names: Benzoic acid, (2-methylphenyl)methyl ester
Inchi: InChI=1S/C15H14O2/c1-12-7-5-6-10-14(12)11-17-15(16)13-8-3-2-4-9-13/h2-10H,11H2,1
InchiKey: NAIUTWJYNXOVNP-UHFFFAOYSA-N
Formula: C15H14O2
SMILES: Cc1ccccc1COC(=O)c1ccccc1
Mol. weight [g/mol]: 226.27
CAS: 80716-36-5

Physical Properties

Property code	Value	Unit	Source
gf	56.69	kJ/mol	Joback Method
hf	-136.14	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	63.35	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.352		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1908.00		NIST Webbook
tb	677.23	K	Joback Method
tc	915.77	K	Joback Method
tf	396.33	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.84	J/mol×K	677.23	Joback Method
cpg	481.42	J/mol×K	716.99	Joback Method
cpg	495.81	J/mol×K	756.74	Joback Method
cpg	509.05	J/mol×K	796.50	Joback Method
cpg	521.19	J/mol×K	836.25	Joback Method
cpg	532.27	J/mol×K	876.01	Joback Method
cpg	542.35	J/mol×K	915.77	Joback Method

dvisc	0.0012300	Pa×s	396.33	Joback Method
dvisc	0.0007015	Pa×s	443.15	Joback Method
dvisc	0.0004454	Pa×s	489.96	Joback Method
dvisc	0.0003061	Pa×s	536.78	Joback Method
dvisc	0.0002234	Pa×s	583.60	Joback Method
dvisc	0.0001709	Pa×s	630.41	Joback Method
dvisc	0.0001356	Pa×s	677.23	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=C80716365&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume