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]: 226.28

Physical Properties

Property code	Value	Unit	Source
af	0.5926		Cheméo Relay (1.0)
gf	56.69	kJ/mol	Joback Method
hf	-178.30	kJ/mol	Cheméo Relay (1.0)
hfus	25.09	kJ/mol	Joback Method
hvap	88.02	kJ/mol	Cheméo Relay (1.0)
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-4.13		Cheméo Relay (1.0)
logp	3.352		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1908.00		NIST Webbook
tb	593.09	K	Cheméo Relay (1.0)
tc	848.90	K	Cheméo Relay (1.0)
tf	301.92	K	Cheméo Relay (1.0)
vc	0.667	m3/kmol	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80716365&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):

Cheméo Relay (1.0, beta):

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

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume