Benzoic acid, 4-methyl-, (4-methylphenyl)methyl ester

Other names: p-Toluic acid, p-methylbenzyl ester
(4-Methylphenyl)methyl 4-methylbenzoate
p-Methylbenzyl p-toluate
4-Methylbenzyl 4-methylbenzoate
p-Toluic acid, p-xylyl ester
(4-methylphenyl)methyl p-toluate

Inchi: InChI=1S/C16H16O2/c1-12-3-7-14(8-4-12)11-18-16(17)15-9-5-13(2)6-10-15/h3-10H,11H

InchiKey: JSMHXVURHYHQGT-UHFFFAOYSA-N

Formula: C16H16O2

SMILES: Cc1ccc(COC(=O)c2ccc(C)cc2)cc1

Mol. weight [g/mol]: 240.30

CAS: 21086-87-3

Physical Properties

Property code	Value	Unit	Source
gf	55.48	kJ/mol	Joback Method
hf	-168.25	kJ/mol	Joback Method
hfus	27.29	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.660		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	705.09	K	Joback Method
tc	939.69	K	Joback Method
tf	420.12	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.05	J/mol×K	705.09	Joback Method
cpg	532.86	J/mol×K	744.19	Joback Method
cpg	547.49	J/mol×K	783.29	Joback Method

cpg	560.99	J/mol×K	822.39	Joback Method
cpg	573.40	J/mol×K	861.49	Joback Method
cpg	584.75	J/mol×K	900.59	Joback Method
cpg	595.10	J/mol×K	939.69	Joback Method
dvisc	0.0009640	Pa×s	420.12	Joback Method
dvisc	0.0005733	Pa×s	467.62	Joback Method
dvisc	0.0003752	Pa×s	515.11	Joback Method
dvisc	0.0002638	Pa×s	562.61	Joback Method
dvisc	0.0001959	Pa×s	610.10	Joback Method
dvisc	0.0001519	Pa×s	657.59	Joback Method
dvisc	0.0001219	Pa×s	705.09	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=C21086873&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