

Benzoic acid, (3-methylphenyl)methyl ester

Inchi:	InChI=1S/C15H14O2/c1-12-6-5-7-13(10-12)11-17-15(16)14-8-3-2-4-9-14/h2-10H,11H2,1
InchiKey:	PNDUDVIQWFVXIO-UHFFFAOYSA-N
Formula:	C15H14O2
SMILES:	<chem>Cc1cccc(COC(=O)c2ccccc2)c1</chem>
Mol. weight [g/mol]:	226.27

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
rinpola	1901.00		NIST Webbook
tb	677.23	K	Joback Method
tc	915.77	K	Joback Method
tf	396.33	K	Joback Method
vc	0.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.84	J/molxK	677.23	Joback Method
cpg	532.27	J/molxK	876.01	Joback Method
cpg	521.19	J/molxK	836.25	Joback Method
cpg	509.05	J/molxK	796.50	Joback Method
cpg	495.81	J/molxK	756.74	Joback Method
cpg	481.42	J/molxK	716.99	Joback Method
cpg	542.35	J/molxK	915.77	Joback Method
dvisc	0.0001356	Paxs	677.23	Joback Method
dvisc	0.0001709	Paxs	630.41	Joback Method

dvisc	0.0002234	Paxs	583.60	Joback Method
dvisc	0.0003061	Paxs	536.78	Joback Method
dvisc	0.0004454	Paxs	489.96	Joback Method
dvisc	0.0007015	Paxs	443.15	Joback Method
dvisc	0.0012300	Paxs	396.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368974&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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