

4-Methoxybenzoic acid, 3-chlorobenzyl ester

Inchi:	InChI=1S/C15H13ClO3/c1-18-14-7-5-12(6-8-14)15(17)19-10-11-3-2-4-13(16)9-11/h2-9H
InchiKey:	RTRWIUZOGDZNEQ-UHFFFAOYSA-N
Formula:	C15H13ClO3
SMILES:	COc1ccc(C(=O)OCc2cccc(Cl)c2)cc1
Mol. weight [g/mol]:	276.71

Physical Properties

Property code	Value	Unit	Source
gf	-69.87	kJ/mol	Joback Method
hf	-295.57	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.706		Crippen Method
mvol	200.240	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	2299.00		NIST Webbook
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tb	742.06	K	Joback Method
tc	980.29	K	Joback Method
tf	461.00	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.23	J/molxK	742.06	Joback Method
cpg	572.47	J/molxK	940.59	Joback Method
cpg	563.22	J/molxK	900.88	Joback Method
cpg	552.89	J/molxK	861.18	Joback Method
cpg	541.47	J/molxK	821.47	Joback Method
cpg	528.92	J/molxK	781.77	Joback Method
cpg	580.67	J/molxK	980.29	Joback Method
dvisc	0.0000975	Paxs	742.06	Joback Method

dvisc	0.0001207	Paxs	695.22	Joback Method
dvisc	0.0001540	Paxs	648.37	Joback Method
dvisc	0.0002042	Paxs	601.53	Joback Method
dvisc	0.0002840	Paxs	554.69	Joback Method
dvisc	0.0004198	Paxs	507.84	Joback Method
dvisc	0.0006716	Paxs	461.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374935&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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