Benzoic acid, (4-chloro-2-methoxyphenyl)methyl ester

Inchi: InChI=1S/C15H13ClO3/c1-18-14-9-13(16)8-7-12(14)10-19-15(17)11-5-3-2-4-6-11/h2-9H,

InchiKey: CZPLZCFGVIJWRQ-UHFFFAOYSA-N

Formula: C15H13ClO3

SMILES: COc1cc(Cl)ccc1COC(=O)c1ccccc1

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
mcvol	200.240	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
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/mol×K	742.06	Joback Method
cpg	572.47	J/mol×K	940.59	Joback Method
cpg	563.22	J/mol×K	900.88	Joback Method
cpg	552.89	J/mol×K	861.18	Joback Method
cpg	541.47	J/mol×K	821.47	Joback Method
cpg	528.92	J/mol×K	781.77	Joback Method
cpg	580.67	J/mol×K	980.29	Joback Method
dvisc	0.0000975	Pa×s	742.06	Joback Method

dvisc	0.0001207	Pa×s	695.22	Joback Method
dvisc	0.0001540	Pa×s	648.37	Joback Method
dvisc	0.0002042	Pa×s	601.53	Joback Method
dvisc	0.0002840	Pa×s	554.69	Joback Method
dvisc	0.0004198	Pa×s	507.84	Joback Method
dvisc	0.0006716	Pa×s	461.00	Joback Method

Sources

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=U368243&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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