

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.23	J/mol×K	742.06	Joback Method
cpg	528.92	J/mol×K	781.77	Joback Method
cpg	541.47	J/mol×K	821.47	Joback Method
cpg	552.89	J/mol×K	861.18	Joback Method
cpg	563.22	J/mol×K	900.88	Joback Method
cpg	572.47	J/mol×K	940.59	Joback Method
cpg	580.67	J/mol×K	980.29	Joback Method
dvisc	0.0006716	Paxs	461.00	Joback Method

dvisc	0.0004198	Paxs	507.84	Joback Method
dvisc	0.0002840	Paxs	554.69	Joback Method
dvisc	0.0002042	Paxs	601.53	Joback Method
dvisc	0.0001540	Paxs	648.37	Joback Method
dvisc	0.0001207	Paxs	695.22	Joback Method
dvisc	0.0000975	Paxs	742.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368243&Units=SI

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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