2-Chlorobenzoic acid, 2-adamantyl ester

Inchi: InChI=1S/C17H19ClO2/c18-15-4-2-1-3-14(15)17(19)20-16-12-6-10-5-11(8-12)9-13(16)7-
InchiKey: HYDIOIONCLEIID-UHFFFAOYSA-N
Formula: C17H19ClO2
SMILES: O=C(OC1C2CC3CC(C2)CC1C3)c1ccccc1Cl
Mol. weight [g/mol]: 290.79

Physical Properties

Property code	Value	Unit	Source
gf	103.92	kJ/mol	Joback Method
hf	-258.13	kJ/mol	Joback Method
hfus	34.87	kJ/mol	Joback Method
hvap	69.21	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.321		Crippen Method
mcvol	213.730	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2214.10		NIST Webbook
rinpol	2214.10		NIST Webbook
tb	748.89	K	Joback Method
tc	989.44	K	Joback Method
tf	464.19	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.32	J/mol×K	748.89	Joback Method
cpg	666.07	J/mol×K	788.98	Joback Method
cpg	683.43	J/mol×K	829.07	Joback Method
cpg	699.52	J/mol×K	869.17	Joback Method
cpg	714.49	J/mol×K	909.26	Joback Method
cpg	728.47	J/mol×K	949.35	Joback Method
cpg	741.58	J/mol×K	989.44	Joback Method
dvisc	0.0040928	Pa×s	464.19	Joback Method

dvisc	0.0036280	Pa×s	511.64	Joback Method
dvisc	0.0032825	Pa×s	559.09	Joback Method
dvisc	0.0030167	Pa×s	606.54	Joback Method
dvisc	0.0028066	Pa×s	653.99	Joback Method
dvisc	0.0026368	Pa×s	701.44	Joback Method
dvisc	0.0024969	Pa×s	748.89	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=U292277&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

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