2-Chlorobenzoic acid, 1-adamantylmethyl ester

Inchi: InChI=1S/C18H21ClO2/c19-16-4-2-1-3-15(16)17(20)21-11-18-8-12-5-13(9-18)7-14(6-12)10-18/h1-4,12-14H,5-11H2

InchiKey: KYXXVMRHEPJPPY-UHFFFAOYSA-N

Formula: C18H21ClO2

SMILES: O=C(OCC12CC3CC(CC(C3)C1)C2)c1ccccc1Cl

Mol. weight [g/mol]: 304.81

Physical Properties

Property code	Value	Unit	Source
gf	114.56	kJ/mol	Joback Method
hf	-243.19	kJ/mol	Joback Method
hfus	30.09	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.713		Crippen Method
mcvol	227.820	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
tb	776.68	K	Joback Method
tc	1020.52	K	Joback Method
tf	503.60	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.60	J/mol×K	776.68	Joback Method
cpg	714.98	J/mol×K	817.32	Joback Method
cpg	733.64	J/mol×K	857.96	Joback Method
cpg	751.86	J/mol×K	898.60	Joback Method
cpg	769.90	J/mol×K	939.24	Joback Method
cpg	788.06	J/mol×K	979.88	Joback Method
cpg	806.60	J/mol×K	1020.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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