2-Chlorobenzoic acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C19H23ClO2/c20-17-4-2-1-3-16(17)18(21)22-6-5-19-10-13-7-14(11-19)9-15(8-

InchiKey: DUPQEGSBYNXUSQ-UHFFFAOYSA-N

Formula: C19H23ClO2

SMILES: O=C(OCCC12CC3CC(CC(C3)C1)C2)c1ccccc1Cl

Mol. weight [g/mol]: 318.84

Physical Properties

Property code	Value	Unit	Source
gf	122.98	kJ/mol	Joback Method
hf	-263.83	kJ/mol	Joback Method
hfus	32.68	kJ/mol	Joback Method
hvap	72.82	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	5.103		Crippen Method
mcvol	241.910	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	2427.40		NIST Webbook
rinpol	2427.40		NIST Webbook
tb	799.56	K	Joback Method
tc	1038.89	K	Joback Method
tf	514.87	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.97	J/mol×K	799.56	Joback Method
cpg	772.76	J/mol×K	839.45	Joback Method
cpg	791.91	J/mol×K	879.34	Joback Method
cpg	810.71	J/mol×K	919.22	Joback Method
cpg	829.41	J/mol×K	959.11	Joback Method
cpg	848.28	J/mol×K	999.00	Joback Method
cpg	867.59	J/mol×K	1038.89	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=U292279&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
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