1-Adamantanecarboxylic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C17H19ClO2/c18-14-1-3-15(4-2-14)20-16(19)17-8-11-5-12(9-17)7-13(6-11)10-

InchiKey: BRFGISNTQUMEQO-UHFFFAOYSA-N

Formula: C17H19ClO2

SMILES: O=C(Oc1ccc(Cl)cc1)C12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 290.79

Physical Properties

Property code	Value	Unit	Source
gf	106.14	kJ/mol	Joback Method
hf	-222.55	kJ/mol	Joback Method
hfus	27.50	kJ/mol	Joback Method
hvap	68.37	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.462		Crippen Method
mcvol	213.730	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	2230.00		NIST Webbook
rinpol	2230.00		NIST Webbook
tb	753.80	K	Joback Method
tc	1002.69	K	Joback Method
tf	492.33	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.38	J/mol×K	753.80	Joback Method
cpg	658.36	J/mol×K	795.28	Joback Method
cpg	676.52	J/mol×K	836.76	Joback Method
cpg	694.14	J/mol×K	878.24	Joback Method
cpg	711.53	J/mol×K	919.72	Joback Method
cpg	728.97	J/mol×K	961.20	Joback Method
cpg	746.75	J/mol×K	1002.69	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307660&Units=SI

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