1-Adamantanecarboxylic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C17H18Cl2O2/c18-14-2-1-13(6-15(14)19)21-16(20)17-7-10-3-11(8-17)5-12(4-1

InchiKey: BQWIKWHHKZSZRP-UHFFFAOYSA-N

Formula: C17H18Cl2O2

SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)C12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 325.23

Physical Properties

Property code	Value	Unit	Source
gf	84.58	kJ/mol	Joback Method
hf	-249.76	kJ/mol	Joback Method
hfus	31.31	kJ/mol	Joback Method
hvap	73.41	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.115		Crippen Method
mcvol	225.970	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	2444.00		NIST Webbook
rinpol	2444.00		NIST Webbook
tb	796.21	K	Joback Method
tc	1047.68	K	Joback Method
tf	534.77	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.54	J/mol×K	796.21	Joback Method
cpg	683.52	J/mol×K	838.12	Joback Method
cpg	700.99	J/mol×K	880.03	Joback Method
cpg	718.25	J/mol×K	921.95	Joback Method
cpg	735.58	J/mol×K	963.86	Joback Method
cpg	753.28	J/mol×K	1005.77	Joback Method
cpg	771.63	J/mol×K	1047.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307664&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