1-Adamantanecarboxylic acid chloride

Other names:	Tricyclo[3.3.1.1(3,7)-]decane-1-carbonyl chloride
	Adamantane-1-carbonyl chloride
	Adamantane-1-carboxylic acid chloride
	1-Adamantanecarbonyl chloride
	1-Adamantanoic acid chloride
	1-Adamantoyl chloride
	1-Adamantylcarbonyl chloride
	tricyclo(3.3.1.1'3,7)decane-1-carbonyl chloride
Inchi:	InChI=1S/C11H15ClO/c12-10(13)11-4-7-1-8(5-11)3-9(2-7)6-11/h7-9H,1-6H2
InchiKey:	MIBQYWIOHFTKHD-UHFFFAOYSA-N
Formula:	C11H15ClO
SMILES:	O=C(Cl)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	198.69
CAS:	2094-72-6

Physical Properties

Property code	Value	Unit	Source
gf	57.84	kJ/mol	Joback Method
hf	-191.55	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	49.66	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.968		Crippen Method
mcvol	147.080	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
tb	562.44	K	Joback Method
tc	796.90	K	Joback Method
tf	363.54	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.11	J/mol×K	562.44	Joback Method

cpg	397.21	J/mol×K	601.52	Joback Method
cpg	413.85	J/mol×K	640.59	Joback Method
cpg	429.24	J/mol×K	679.67	Joback Method
cpg	443.64	J/mol×K	718.75	Joback Method
cpg	457.28	J/mol×K	757.82	Joback Method
cpg	470.39	J/mol×K	796.90	Joback Method

Sources

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=C2094726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume