

Adamantane-1-carboxylic acid, tert.-butyl ester

Inchi:	InChI=1S/C15H24O2/c1-14(2,3)17-13(16)15-7-10-4-11(8-15)6-12(5-10)9-15/h10-12H,4-9
InchiKey:	QBOVXIMGMVOPQK-UHFFFAOYSA-N
Formula:	C15H24O2
SMILES:	CC(C)(C)OC(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	1.29	kJ/mol	Joback Method
hf	-399.34	kJ/mol	Joback Method
hfus	17.06	kJ/mol	Joback Method
hvap	55.30	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.545		Crippen Method
mcvol	197.070	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1556.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1896.00		NIST Webbook
tb	635.72	K	Joback Method
tc	859.57	K	Joback Method
tf	403.35	K	Joback Method
vc	0.749	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.47	J/molxK	635.72	Joback Method
cpg	604.67	J/molxK	673.03	Joback Method

cpg	624.51	J/mol×K	710.34	Joback Method
cpg	643.22	J/mol×K	747.65	Joback Method
cpg	661.02	J/mol×K	784.95	Joback Method
cpg	678.14	J/mol×K	822.26	Joback Method
cpg	694.80	J/mol×K	859.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
r ipol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/84-889-3/Adamantane-1-carboxylic-acid-tert-butyl-ester.pdf>

Generated by Cheméo on 2024-04-27 14:12:21.544571787 +0000 UTC m=+16516390.465149102.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.