

1-Adamantanecarboxylic acid, isopropyl ester

Other names:	Adamantane-1-carboxylic acid, isopropyl ester
Inchi:	InChI=1S/C14H22O2/c1-9(2)16-13(15)14-6-10-3-11(7-14)5-12(4-10)8-14/h9-12H,3-8H2,
InchiKey:	PHSXXMGYVSYRPF-UHFFFAOYSA-N
Formula:	C14H22O2
SMILES:	CC(C)OC(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	222.32
CAS:	24556-16-9

Physical Properties

Property code	Value	Unit	Source
gf	-12.41	kJ/mol	Joback Method
hf	-375.23	kJ/mol	Joback Method
hfus	18.36	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.154		Crippen Method
mcvol	182.980	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1568.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1532.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1894.00		NIST Webbook
tb	615.63	K	Joback Method
tc	835.19	K	Joback Method
tf	374.66	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.66	J/molxK	615.63	Joback Method

cpg	548.03	J/mol×K	652.22	Joback Method
cpg	567.13	J/mol×K	688.82	Joback Method
cpg	585.15	J/mol×K	725.41	Joback Method
cpg	602.28	J/mol×K	762.00	Joback Method
cpg	618.70	J/mol×K	798.60	Joback Method
cpg	634.60	J/mol×K	835.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24556169&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
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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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