

1-Adamantanecarboxylic acid, isobutyl ester

Other names:	Adamantane-1-carboxylic acid, isobutyl ester
Inchi:	InChI=1S/C15H24O2/c1-10(2)9-17-14(16)15-6-11-3-12(7-15)5-13(4-11)8-15/h10-13H,3-9
InchiKey:	RQZHXUPVGBYMHW-UHFFFAOYSA-N
Formula:	C15H24O2
SMILES:	CC(C)COC(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	236.35
CAS:	24556-18-1

Physical Properties

Property code	Value	Unit	Source
gf	-3.99	kJ/mol	Joback Method
hf	-395.87	kJ/mol	Joback Method
hfus	20.95	kJ/mol	Joback Method
hvap	56.20	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.402		Crippen Method
mcvol	197.070	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1658.00		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2082.00		NIST Webbook
ripol	2060.00		NIST Webbook
tb	638.51	K	Joback Method
tc	854.28	K	Joback Method
tf	385.93	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.22	J/molxK	638.51	Joback Method

cpg	601.85	J/mol×K	674.47	Joback Method
cpg	621.29	J/mol×K	710.43	Joback Method
cpg	639.71	J/mol×K	746.39	Joback Method
cpg	657.31	J/mol×K	782.36	Joback Method
cpg	674.24	J/mol×K	818.32	Joback Method
cpg	690.71	J/mol×K	854.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24556181&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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