2-Ethoxycarbonyladamantane

Other names: Adamantane-2-carboxylic acid, ethyl ester
Inchi: InChI=1S/C13H20O2/c1-2-15-13(14)12-10-4-8-3-9(6-10)7-11(12)5-8/h8-12H,2-7H2,1H3
InchiKey: VYLWDQILLRTFOG-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CCOC(=O)C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-20.61	kJ/mol	Joback Method
hf	-384.89	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	52.98	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.622		Crippen Method
mcvol	168.890	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1542.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1566.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1999.00		NIST Webbook
ripol	1976.00		NIST Webbook
ripol	1954.00		NIST Webbook
tb	588.28	K	Joback Method
tc	798.95	K	Joback Method
tf	350.25	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.03	J/mol×K	588.28	Joback Method

cpg	498.32	J/mol×K	623.39	Joback Method
cpg	517.33	J/mol×K	658.50	Joback Method
cpg	535.17	J/mol×K	693.61	Joback Method
cpg	551.89	J/mol×K	728.72	Joback Method
cpg	567.57	J/mol×K	763.83	Joback Method
cpg	582.29	J/mol×K	798.95	Joback Method
dvisc	0.0023748	Pa×s	350.25	Joback Method
dvisc	0.0023248	Pa×s	389.92	Joback Method
dvisc	0.0022848	Pa×s	429.59	Joback Method
dvisc	0.0022521	Pa×s	469.26	Joback Method
dvisc	0.0022249	Pa×s	508.94	Joback Method
dvisc	0.0022018	Pa×s	548.61	Joback Method
dvisc	0.0021821	Pa×s	588.28	Joback Method

Sources

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=U306448&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume