Acetoxyacetic acid, 2-adamantyl ester

Inchi: InChI=1S/C14H20O4/c1-8(15)17-7-13(16)18-14-11-3-9-2-10(5-11)6-12(14)4-9/h9-12,14H
InchiKey: USARLLDMEVXLIO-UHFFFAOYSA-N
Formula: C14H20O4
SMILES: CC(=O)OCC(=O)OC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
gf	-246.11	kJ/mol	Joback Method
hf	-650.33	kJ/mol	Joback Method
hfus	32.04	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.917		Crippen Method
mcvol	190.420	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1788.00		NIST Webbook
rinpol	1788.00		NIST Webbook
tb	687.45	K	Joback Method
tc	899.32	K	Joback Method
tf	433.68	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.39	J/mol×K	687.45	Joback Method
cpg	603.54	J/mol×K	722.76	Joback Method
cpg	620.54	J/mol×K	758.07	Joback Method
cpg	636.44	J/mol×K	793.38	Joback Method
cpg	651.32	J/mol×K	828.70	Joback Method
cpg	665.23	J/mol×K	864.01	Joback Method
cpg	678.24	J/mol×K	899.32	Joback Method
dvisc	0.0038446	Pa×s	433.68	Joback Method

dvisc	0.0034450	Pa×s	475.97	Joback Method
dvisc	0.0031426	Pa×s	518.27	Joback Method
dvisc	0.0029069	Pa×s	560.57	Joback Method
dvisc	0.0027184	Pa×s	602.86	Joback Method
dvisc	0.0025645	Pa×s	645.15	Joback Method
dvisc	0.0024368	Pa×s	687.45	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=U308315&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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