Acetoxyacetic acid, 1-adamantylmethyl ester

Inchi: InChI=1S/C15H22O4/c1-10(16)18-8-14(17)19-9-15-5-11-2-12(6-15)4-13(3-11)7-15/h11-1
InchiKey: UMSIGAOSPZWFSL-UHFFFAOYSA-N
Formula: C15H22O4
SMILES: CC(=O)OCC(=O)OCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 266.33

Physical Properties

Property code	Value	Unit	Source
gf	-235.47	kJ/mol	Joback Method
hf	-635.39	kJ/mol	Joback Method
hfus	27.26	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.309		Crippen Method
mcvol	204.510	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1884.00		NIST Webbook
rinpol	1884.00		NIST Webbook
tb	715.24	K	Joback Method
tc	930.92	K	Joback Method
tf	473.09	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.69	J/mol×K	715.24	Joback Method
cpg	651.83	J/mol×K	751.19	Joback Method
cpg	669.14	J/mol×K	787.13	Joback Method
cpg	685.77	J/mol×K	823.08	Joback Method
cpg	701.88	J/mol×K	859.02	Joback Method
cpg	717.65	J/mol×K	894.97	Joback Method
cpg	733.22	J/mol×K	930.92	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=U308316&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
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