Acetoxyacetic acid, 2-naphthyl ester

Inchi: InChI=1S/C14H12O4/c1-10(15)17-9-14(16)18-13-7-6-11-4-2-3-5-12(11)8-13/h2-8H,9H2,
InchiKey: QEWYPKWCQKJOGE-UHFFFAOYSA-N
Formula: C14H12O4
SMILES: CC(=O)OCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 244.24

Physical Properties

Property code	Value	Unit	Source
gf	-191.41	kJ/mol	Joback Method
hf	-405.76	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	69.65	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.308		Crippen Method
mcvol	179.780	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook
tb	722.94	K	Joback Method
tc	951.99	K	Joback Method
tf	463.50	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.10	J/mol×K	722.94	Joback Method
cpg	485.71	J/mol×K	761.12	Joback Method
cpg	497.36	J/mol×K	799.29	Joback Method
cpg	508.09	J/mol×K	837.47	Joback Method
cpg	517.94	J/mol×K	875.64	Joback Method
cpg	526.93	J/mol×K	913.82	Joback Method
cpg	535.11	J/mol×K	951.99	Joback Method
dvisc	0.0010602	Pa×s	463.50	Joback Method

dvisc	0.0007269	Pa×s	506.74	Joback Method
dvisc	0.0005289	Pa×s	549.98	Joback Method
dvisc	0.0004031	Pa×s	593.22	Joback Method
dvisc	0.0003187	Pa×s	636.46	Joback Method
dvisc	0.0002597	Pa×s	679.70	Joback Method
dvisc	0.0002168	Pa×s	722.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307546&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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