

Acetoxyacetic acid, 1-naphthyl ester

Inchi:	InChI=1S/C14H12O4/c1-10(15)17-9-14(16)18-13-8-4-6-11-5-2-3-7-12(11)13/h2-8H,9H2,
InchiKey:	NXKZMCDDKZZDHM-UHFFFAOYSA-N
Formula:	C14H12O4
SMILES:	CC(=O)OCC(=O)Oc1cccc2ccccc12
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
mvol	179.780	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1884.00		NIST Webbook
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tb	722.94	K	Joback Method
tc	951.99	K	Joback Method
tf	463.50	K	Joback Method
vc	0.681	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.10	J/mol×K	722.94	Joback Method
cpg	526.93	J/mol×K	913.82	Joback Method
cpg	517.94	J/mol×K	875.64	Joback Method
cpg	508.09	J/mol×K	837.47	Joback Method
cpg	497.36	J/mol×K	799.29	Joback Method
cpg	485.71	J/mol×K	761.12	Joback Method
cpg	535.11	J/mol×K	951.99	Joback Method
dvisc	0.0002168	Paxs	722.94	Joback Method

dvisc	0.0002597	Paxs	679.70	Joback Method
dvisc	0.0003187	Paxs	636.46	Joback Method
dvisc	0.0004031	Paxs	593.22	Joback Method
dvisc	0.0005289	Paxs	549.98	Joback Method
dvisc	0.0007269	Paxs	506.74	Joback Method
dvisc	0.0010602	Paxs	463.50	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=U308344&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

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