

Acetoxyacetic acid, 3-ethylphenyl ester

Inchi:	InChI=1S/C12H14O4/c1-3-10-5-4-6-11(7-10)16-12(14)8-15-9(2)13/h4-7H,3,8H2,1-2H3
InchiKey:	FMTUBNZETJPNHI-UHFFFAOYSA-N
Formula:	C12H14O4
SMILES:	CCc1cccc(OC(=O)COC(C)=O)c1
Mol. weight [g/mol]:	222.24

Physical Properties

Property code	Value	Unit	Source
gf	-314.90	kJ/mol	Joback Method
hf	-555.55	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	63.56	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.717		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1633.00		NIST Webbook
tb	658.20	K	Joback Method
tc	870.02	K	Joback Method
tf	408.26	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.51	J/molxK	658.20	Joback Method
cpg	495.18	J/molxK	834.72	Joback Method
cpg	485.06	J/molxK	799.41	Joback Method
cpg	474.13	J/molxK	764.11	Joback Method
cpg	462.40	J/molxK	728.81	Joback Method
cpg	449.86	J/molxK	693.50	Joback Method
cpg	504.49	J/molxK	870.02	Joback Method
dvisc	0.0001492	Paxs	658.20	Joback Method
dvisc	0.0001863	Paxs	616.54	Joback Method

dvisc	0.0002401	Paxs	574.89	Joback Method
dvisc	0.0003219	Paxs	533.23	Joback Method
dvisc	0.0004537	Paxs	491.57	Joback Method
dvisc	0.0006814	Paxs	449.92	Joback Method
dvisc	0.0011118	Paxs	408.26	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=U355699&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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