

Acetoxyacetic acid, 3-methylphenyl ester

Inchi:	InChI=1S/C11H12O4/c1-8-4-3-5-10(6-8)15-11(13)7-14-9(2)12/h3-6H,7H2,1-2H3
InchiKey:	YRYVECQLYXIZKI-UHFFFAOYSA-N
Formula:	C11H12O4
SMILES:	CC(=O)OCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	208.21

Physical Properties

Property code	Value	Unit	Source
gf	-323.32	kJ/mol	Joback Method
hf	-534.91	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	61.33	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.464		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1487.00		NIST Webbook
tb	635.32	K	Joback Method
tc	850.61	K	Joback Method
tf	396.99	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.89	J/molxK	635.32	Joback Method
cpg	399.58	J/molxK	671.20	Joback Method
cpg	411.51	J/molxK	707.08	Joback Method
cpg	422.68	J/molxK	742.97	Joback Method
cpg	433.09	J/molxK	778.85	Joback Method
cpg	442.73	J/molxK	814.73	Joback Method
cpg	451.61	J/molxK	850.61	Joback Method
dvisc	0.0011650	Paxs	396.99	Joback Method
dvisc	0.0007259	Paxs	436.71	Joback Method

dvisc	0.0004894	Paxs	476.43	Joback Method
dvisc	0.0003506	Paxs	516.15	Joback Method
dvisc	0.0002634	Paxs	555.88	Joback Method
dvisc	0.0002056	Paxs	595.60	Joback Method
dvisc	0.0001656	Paxs	635.32	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=U307539&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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