

Acetic acid, 2,4,6-trimethylbenzyl ester

Inchi:	InChI=1S/C12H16O2/c1-8-5-9(2)12(10(3)6-8)7-14-11(4)13/h5-6H,7H2,1-4H3
InchiKey:	KKRQFZYXQHIORO-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CC(=O)OCc1c(C)cc(C)cc1C
Mol. weight [g/mol]:	192.25
CAS:	63548-92-5

Physical Properties

Property code	Value	Unit	Source
gf	-100.24	kJ/mol	Joback Method
hf	-333.69	kJ/mol	Joback Method
hfus	22.50	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.675		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
tb	591.87	K	Joback Method
tc	800.82	K	Joback Method
tf	361.14	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.00	J/mol×K	591.87	Joback Method
cpg	407.43	J/mol×K	626.70	Joback Method
cpg	421.16	J/mol×K	661.52	Joback Method
cpg	434.17	J/mol×K	696.35	Joback Method
cpg	446.48	J/mol×K	731.17	Joback Method
cpg	458.09	J/mol×K	766.00	Joback Method
cpg	469.00	J/mol×K	800.82	Joback Method
dvisc	0.0010751	Pa×s	361.14	Joback Method
dvisc	0.0006856	Pa×s	399.60	Joback Method

dvisc	0.0004732	Pa×s	438.05	Joback Method
dvisc	0.0003467	Pa×s	476.50	Joback Method
dvisc	0.0002661	Pa×s	514.96	Joback Method
dvisc	0.0002119	Pa×s	553.41	Joback Method
dvisc	0.0001738	Pa×s	591.87	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=C63548925&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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