

Succinic acid, ethyl 3-methylbenzyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C14H18O4/c1-3-17-13(15)7-8-14(16)18-10-12-6-4-5-11(2)9-12/h4-6,9H,3,7-8,1

OBNXSNFGQMLMLS-UHFFFAOYSA-N

C14H18O4

CCOC(=O)CCC(=O)OCc1cccc(C)c1

250.29

Physical Properties

Property code	Value	Unit	Source
gf	-298.06	kJ/mol	Joback Method
hf	-596.83	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	68.01	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.382		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1836.00		NIST Webbook
rinpol	1836.00		NIST Webbook
tb	703.96	K	Joback Method
tc	909.90	K	Joback Method
tf	430.80	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.98	J/mol×K	703.96	Joback Method
cpg	554.36	J/mol×K	738.28	Joback Method
cpg	567.84	J/mol×K	772.61	Joback Method
cpg	580.44	J/mol×K	806.93	Joback Method
cpg	592.16	J/mol×K	841.25	Joback Method
cpg	603.00	J/mol×K	875.58	Joback Method
cpg	612.97	J/mol×K	909.90	Joback Method
dvisc	0.0009874	Pa×s	430.80	Joback Method

dvisc	0.0005866	Pa×s	476.33	Joback Method
dvisc	0.0003816	Pa×s	521.85	Joback Method
dvisc	0.0002660	Pa×s	567.38	Joback Method
dvisc	0.0001956	Pa×s	612.91	Joback Method
dvisc	0.0001501	Pa×s	658.43	Joback Method
dvisc	0.0001192	Pa×s	703.96	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U382388&Units=SI

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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