

Succinic acid, ethyl 4-methylbenzyl ester

Inchi:	InChI=1S/C14H18O4/c1-3-17-13(15)8-9-14(16)18-10-12-6-4-11(2)5-7-12/h4-7H,3,8-10H
InchiKey:	DDAYJJCKPVVKHU-UHFFFAOYSA-N
Formula:	C14H18O4
SMILES:	CCOC(=O)CCC(=O)OCc1ccc(C)cc1
Mol. weight [g/mol]:	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	1848.00		NIST Webbook
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tb	703.96	K	Joback Method
tc	909.90	K	Joback Method
tf	430.80	K	Joback Method
vc	0.759	m ³ /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	Paxs	430.80	Joback Method

dvisc	0.0005866	Paxs	476.33	Joback Method
dvisc	0.0003816	Paxs	521.85	Joback Method
dvisc	0.0002660	Paxs	567.38	Joback Method
dvisc	0.0001956	Paxs	612.91	Joback Method
dvisc	0.0001501	Paxs	658.43	Joback Method
dvisc	0.0001192	Paxs	703.96	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=U381050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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