

Diglycolic acid, ethyl 4-methoxyphenyl ester

Inchi:	InChI=1S/C13H16O6/c1-3-18-12(14)8-17-9-13(15)19-11-6-4-10(16-2)5-7-11/h4-7H,3,8-9
InchiKey:	LDHMSNBKKBPUOH-UHFFFAOYSA-N
Formula:	C13H16O6
SMILES:	CCOC(=O)COCC(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]:	268.26

Physical Properties

Property code	Value	Unit	Source
gf	-516.48	kJ/mol	Joback Method
hf	-840.63	kJ/mol	Joback Method
hfus	31.03	kJ/mol	Joback Method
hvap	70.60	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.180		Crippen Method
mcvol	196.890	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	2488.00		NIST Webbook
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tb	725.92	K	Joback Method
tc	931.20	K	Joback Method
tf	463.99	K	Joback Method
vc	0.740	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.65	J/molxK	725.92	Joback Method
cpg	553.00	J/molxK	760.13	Joback Method
cpg	565.47	J/molxK	794.35	Joback Method
cpg	577.03	J/molxK	828.56	Joback Method
cpg	587.66	J/molxK	862.77	Joback Method
cpg	597.33	J/molxK	896.98	Joback Method
cpg	606.03	J/molxK	931.20	Joback Method
dvisc	0.0005583	Paxs	463.99	Joback Method

dvisc	0.0003515	Paxs	507.65	Joback Method
dvisc	0.0002381	Paxs	551.30	Joback Method
dvisc	0.0001707	Paxs	594.96	Joback Method
dvisc	0.0001281	Paxs	638.61	Joback Method
dvisc	0.0000998	Paxs	682.27	Joback Method
dvisc	0.0000801	Paxs	725.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381883&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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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