

Diglycolic acid, ethyl 4-methoxybenzyl ester

Inchi:	InChI=1S/C14H18O6/c1-3-19-13(15)9-18-10-14(16)20-8-11-4-6-12(17-2)7-5-11/h4-7H,3,
InchiKey:	SNBHHPYAGWSTKL-UHFFFAOYSA-N
Formula:	C14H18O6
SMILES:	CCOC(=O)COCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]:	282.29

Physical Properties

Property code	Value	Unit	Source
gf	-508.06	kJ/mol	Joback Method
hf	-861.27	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	72.83	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.318		Crippen Method
mcvol	210.980	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	2675.00		NIST Webbook
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tb	748.80	K	Joback Method
tc	952.07	K	Joback Method
tf	475.26	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.40	J/molxK	748.80	Joback Method
cpg	652.51	J/molxK	918.19	Joback Method
cpg	642.65	J/molxK	884.31	Joback Method
cpg	631.79	J/molxK	850.44	Joback Method
cpg	619.95	J/molxK	816.56	Joback Method
cpg	607.15	J/molxK	782.68	Joback Method
cpg	661.35	J/molxK	952.07	Joback Method
dvisc	0.0000705	Paxs	748.80	Joback Method

dvisc	0.0000882	Paxs	703.21	Joback Method
dvisc	0.0001139	Paxs	657.62	Joback Method
dvisc	0.0001528	Paxs	612.03	Joback Method
dvisc	0.0002148	Paxs	566.44	Joback Method
dvisc	0.0003206	Paxs	520.85	Joback Method
dvisc	0.0005167	Paxs	475.26	Joback Method

Sources

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=U382247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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