Diglycolic acid, ethyl 4-nitrophenyl ester

Inchi: InChI=1S/C12H13NO7/c1-2-19-11(14)7-18-8-12(15)20-10-5-3-9(4-6-10)13(16)17/h3-6H,
InchiKey: PMTHQAUIUHXPOO-UHFFFAOYSA-N
Formula: C12H13NO7
SMILES: CCOC(=O)COCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 283.23

Physical Properties

Property code	Value	Unit	Source
gf	-384.35	kJ/mol	Joback Method
hf	-698.53	kJ/mol	Joback Method
hfus	38.61	kJ/mol	Joback Method
hvap	82.56	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.080		Crippen Method
mcvol	194.350	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	2699.00		NIST Webbook
tb	832.46	K	Joback Method
tc	1061.36	K	Joback Method
tf	574.10	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.03	J/mol×K	832.46	Joback Method
cpg	568.71	J/mol×K	870.61	Joback Method
cpg	578.28	J/mol×K	908.76	Joback Method
cpg	586.74	J/mol×K	946.91	Joback Method
cpg	594.06	J/mol×K	985.06	Joback Method
cpg	600.25	J/mol×K	1023.21	Joback Method
cpg	605.29	J/mol×K	1061.36	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=U381882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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