Diglycolic acid, 4-cyanophenyl ethyl ester

Inchi: InChI=1S/C13H13NO5/c1-2-18-12(15)8-17-9-13(16)19-11-5-3-10(7-14)4-6-11/h3-6H,2,8-
InchiKey: SJDVORNDWQRYOC-UHFFFAOYSA-N
Formula: C13H13NO5
SMILES: CCOC(=O)COCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 263.25

Physical Properties

Property code	Value	Unit	Source
gf	-278.30	kJ/mol	Joback Method
hf	-543.53	kJ/mol	Joback Method
hfus	31.35	kJ/mol	Joback Method
hvap	78.67	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.043		Crippen Method
mcvol	192.400	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	2553.00		NIST Webbook
rinpol	2553.00		NIST Webbook
tb	805.58	K	Joback Method
tc	1024.36	K	Joback Method
tf	506.75	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.68	J/mol×K	805.58	Joback Method
cpg	543.36	J/mol×K	842.04	Joback Method
cpg	553.10	J/mol×K	878.51	Joback Method
cpg	561.86	J/mol×K	914.97	Joback Method
cpg	569.64	J/mol×K	951.43	Joback Method
cpg	576.43	J/mol×K	987.89	Joback Method
cpg	582.21	J/mol×K	1024.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381966&Units=SI
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

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

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