Diglycolic acid, butyl 4-cyanophenyl ester

Inchi: InChI=1S/C15H17NO5/c1-2-3-8-20-14(17)10-19-11-15(18)21-13-6-4-12(9-16)5-7-13/h4-
InchiKey: KHDUPPSQPOBQGB-UHFFFAOYSA-N
Formula: C15H17NO5
SMILES: CCCCOC(=O)COCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 291.30

Physical Properties

Property code	Value	Unit	Source
gf	-261.46	kJ/mol	Joback Method
hf	-584.81	kJ/mol	Joback Method
hfus	36.53	kJ/mol	Joback Method
hvap	83.12	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.824		Crippen Method
mcvol	220.580	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2803.00		NIST Webbook
rinpol	2803.00		NIST Webbook
tb	851.34	K	Joback Method
tc	1066.61	K	Joback Method
tf	529.29	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.70	J/mol×K	851.34	Joback Method
cpg	653.01	J/mol×K	887.22	Joback Method
cpg	663.26	J/mol×K	923.10	Joback Method
cpg	672.45	J/mol×K	958.97	Joback Method
cpg	680.57	J/mol×K	994.85	Joback Method
cpg	687.61	J/mol×K	1030.73	Joback Method
cpg	693.58	J/mol×K	1066.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381967&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