Succinic acid, 4-cyanophenyl 2-methoxyethyl ester

Inchi: InChI=1S/C14H15NO5/c1-18-8-9-19-13(16)6-7-14(17)20-12-4-2-11(10-15)3-5-12/h2-5H,
InchiKey: WQRUEPQARURRPN-UHFFFAOYSA-N
Formula: C14H15NO5
SMILES: COCCOC(=O)CCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 277.27

Physical Properties

Property code	Value	Unit	Source
gf	-269.88	kJ/mol	Joback Method
hf	-564.17	kJ/mol	Joback Method
hfus	33.94	kJ/mol	Joback Method
hvap	80.90	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.433		Crippen Method
mcvol	206.490	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	2228.00		NIST Webbook
tb	828.46	K	Joback Method
tc	1045.17	K	Joback Method
tf	518.02	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.72	J/mol×K	828.46	Joback Method
cpg	597.75	J/mol×K	864.58	Joback Method
cpg	607.77	J/mol×K	900.70	Joback Method
cpg	616.77	J/mol×K	936.81	Joback Method
cpg	624.75	J/mol×K	972.93	Joback Method
cpg	631.70	J/mol×K	1009.05	Joback Method
cpg	637.60	J/mol×K	1045.17	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360701&Units=SI

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