Sebacic acid, 4-cyanophenyl ethyl ester

Inchi: InChI=1S/C19H25NO4/c1-2-23-18(21)9-7-5-3-4-6-8-10-19(22)24-17-13-11-16(15-20)12-
InchiKey: HOIBETSIIPOZNB-UHFFFAOYSA-N
Formula: C19H25NO4
SMILES: CCOC(=O)CCCCCCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 331.41

Physical Properties

Property code	Value	Unit	Source
gf	-122.78	kJ/mol	Joback Method
hf	-535.15	kJ/mol	Joback Method
hfus	45.70	kJ/mol	Joback Method
hvap	89.62	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.148		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	2682.00		NIST Webbook
tb	920.44	K	Joback Method
tc	1135.27	K	Joback Method
tf	552.14	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.80	J/mol×K	920.44	Joback Method
cpg	855.52	J/mol×K	956.24	Joback Method
cpg	867.09	J/mol×K	992.05	Joback Method
cpg	877.53	J/mol×K	1027.85	Joback Method
cpg	886.87	J/mol×K	1063.66	Joback Method
cpg	895.11	J/mol×K	1099.46	Joback Method
cpg	902.29	J/mol×K	1135.27	Joback Method

Sources

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=U354439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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