Sebacic acid, 4-cyanophenyl isohexyl ester

Inchi: InChI=1S/C23H33NO4/c1-19(2)10-9-17-27-22(25)11-7-5-3-4-6-8-12-23(26)28-21-15-13-
InchiKey: WNVRUXYIVAJUMN-UHFFFAOYSA-N
Formula: C23H33NO4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 387.51

Physical Properties

Property code	Value	Unit	Source
gf	-91.54	kJ/mol	Joback Method
hf	-622.99	kJ/mol	Joback Method
hfus	52.53	kJ/mol	Joback Method
hvap	98.13	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.564		Crippen Method
mcvol	327.430	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	3067.00		NIST Webbook
tb	1011.52	K	Joback Method
tc	1238.52	K	Joback Method
tf	582.22	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1080.79	J/mol×K	1011.52	Joback Method
cpg	1094.21	J/mol×K	1049.35	Joback Method
cpg	1106.20	J/mol×K	1087.19	Joback Method
cpg	1116.80	J/mol×K	1125.02	Joback Method
cpg	1126.06	J/mol×K	1162.85	Joback Method
cpg	1134.01	J/mol×K	1200.69	Joback Method
cpg	1140.70	J/mol×K	1238.52	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=U354444&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