Sebacic acid, 4-cyanophenyl pentyl ester

Inchi: InChI=1S/C22H31NO4/c1-2-3-10-17-26-21(24)11-8-6-4-5-7-9-12-22(25)27-20-15-13-19(
InchiKey: UXEAQFPKSNATEX-UHFFFAOYSA-N
Formula: C22H31NO4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 373.49

Physical Properties

Property code	Value	Unit	Source
gf	-97.52	kJ/mol	Joback Method
hf	-597.07	kJ/mol	Joback Method
hfus	53.47	kJ/mol	Joback Method
hvap	96.29	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.318		Crippen Method
mcvol	313.340	ml/mol	McGowan Method
pc	1151.44	kPa	Joback Method
rinpol	3002.00		NIST Webbook
tb	989.08	K	Joback Method
tc	1211.57	K	Joback Method
tf	585.95	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.23	J/mol×K	989.08	Joback Method
cpg	1033.52	J/mol×K	1026.16	Joback Method
cpg	1045.48	J/mol×K	1063.24	Joback Method
cpg	1056.13	J/mol×K	1100.32	Joback Method
cpg	1065.52	J/mol×K	1137.40	Joback Method
cpg	1073.69	J/mol×K	1174.48	Joback Method
cpg	1080.66	J/mol×K	1211.57	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=U354443&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