Sebacic acid, 4-cyanophenyl heptyl ester

Inchi: InChI=1S/C24H35NO4/c1-2-3-4-9-12-19-28-23(26)13-10-7-5-6-8-11-14-24(27)29-22-17-
InchiKey: UZMKZYVIGOJPTQ-UHFFFAOYSA-N
Formula: C24H35NO4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 401.54

Physical Properties

Property code	Value	Unit	Source
gf	-80.68	kJ/mol	Joback Method
hf	-638.35	kJ/mol	Joback Method
hfus	58.65	kJ/mol	Joback Method
hvap	100.75	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.098		Crippen Method
mcvol	341.520	ml/mol	McGowan Method
pc	1014.89	kPa	Joback Method
rinpol	3214.00		NIST Webbook
tb	1034.84	K	Joback Method
tc	1267.37	K	Joback Method
tf	608.49	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1141.10	J/mol×K	1034.84	Joback Method
cpg	1154.79	J/mol×K	1073.60	Joback Method
cpg	1166.98	J/mol×K	1112.35	Joback Method
cpg	1177.71	J/mol×K	1151.11	Joback Method
cpg	1187.03	J/mol×K	1189.86	Joback Method
cpg	1195.00	J/mol×K	1228.62	Joback Method
cpg	1201.65	J/mol×K	1267.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354446&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