Sebacic acid, 4-cyanophenyl nonyl ester

Inchi: InChI=1S/C26H39NO4/c1-2-3-4-5-8-11-14-21-30-25(28)15-12-9-6-7-10-13-16-26(29)31-
InchiKey: UWBDSIDBVCBNIC-UHFFFAOYSA-N
Formula: C26H39NO4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 429.59

Physical Properties

Property code	Value	Unit	Source
gf	-63.84	kJ/mol	Joback Method
hf	-679.63	kJ/mol	Joback Method
hfus	63.83	kJ/mol	Joback Method
hvap	105.20	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	6.878		Crippen Method
mcvol	369.700	ml/mol	McGowan Method
pc	901.26	kPa	Joback Method
rinpol	3423.00		NIST Webbook
rinpol	3423.00		NIST Webbook
tb	1080.60	K	Joback Method
tc	1327.80	K	Joback Method
tf	631.03	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1263.59	J/mol×K	1080.60	Joback Method
cpg	1277.73	J/mol×K	1121.80	Joback Method
cpg	1290.15	J/mol×K	1163.00	Joback Method
cpg	1300.90	J/mol×K	1204.20	Joback Method
cpg	1310.07	J/mol×K	1245.40	Joback Method
cpg	1317.71	J/mol×K	1286.60	Joback Method
cpg	1323.89	J/mol×K	1327.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354448&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