Sebacic acid, 4-cyanophenyl isobutyl ester

Inchi: InChI=1S/C21H29NO4/c1-17(2)16-25-20(23)9-7-5-3-4-6-8-10-21(24)26-19-13-11-18(15-
InchiKey: MJHKKBRQPXNGSC-UHFFFAOYSA-N
Formula: C21H29NO4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 359.46

Physical Properties

Property code	Value	Unit	Source
gf	-108.38	kJ/mol	Joback Method
hf	-581.71	kJ/mol	Joback Method
hfus	47.35	kJ/mol	Joback Method
hvap	93.68	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.784		Crippen Method
mcvol	299.250	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	2837.00		NIST Webbook
rinpol	2837.00		NIST Webbook
tb	965.76	K	Joback Method
tc	1185.59	K	Joback Method
tf	559.68	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	960.95	J/mol×K	965.76	Joback Method
cpg	974.05	J/mol×K	1002.40	Joback Method
cpg	985.86	J/mol×K	1039.04	Joback Method
cpg	996.41	J/mol×K	1075.68	Joback Method
cpg	1005.73	J/mol×K	1112.32	Joback Method
cpg	1013.86	J/mol×K	1148.96	Joback Method
cpg	1020.82	J/mol×K	1185.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354441&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