Sebacic acid, butyl 4-cyanophenyl ester

Inchi: InChI=1S/C21H29NO4/c1-2-3-16-25-20(23)10-8-6-4-5-7-9-11-21(24)26-19-14-12-18(17-
InchiKey: KSTMNESTIFNQNS-UHFFFAOYSA-N
Formula: C21H29NO4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 359.46

Physical Properties

Property code	Value	Unit	Source
gf	-105.94	kJ/mol	Joback Method
hf	-576.43	kJ/mol	Joback Method
hfus	50.88	kJ/mol	Joback Method
hvap	94.07	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	4.928		Crippen Method
mcvol	299.250	ml/mol	McGowan Method
pc	1230.28	kPa	Joback Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
tb	966.20	K	Joback Method
tc	1185.21	K	Joback Method
tf	574.68	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	960.51	J/mol×K	966.20	Joback Method
cpg	973.62	J/mol×K	1002.70	Joback Method
cpg	985.45	J/mol×K	1039.20	Joback Method
cpg	996.05	J/mol×K	1075.70	Joback Method
cpg	1005.45	J/mol×K	1112.21	Joback Method
cpg	1013.67	J/mol×K	1148.71	Joback Method
cpg	1020.74	J/mol×K	1185.21	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=U354442&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