Sebacic acid, 4-cyanophenyl propyl ester

Inchi: InChI=1S/C20H27NO4/c1-2-15-24-19(22)9-7-5-3-4-6-8-10-20(23)25-18-13-11-17(16-21)
InchiKey: DBPHHYFCLLFMEG-UHFFFAOYSA-N
Formula: C20H27NO4
SMILES: CCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 345.43

Physical Properties

Property code	Value	Unit	Source
gf	-114.36	kJ/mol	Joback Method
hf	-555.79	kJ/mol	Joback Method
hfus	48.29	kJ/mol	Joback Method
hvap	91.84	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.538		Crippen Method
mcvol	285.160	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	2780.00		NIST Webbook
tb	943.32	K	Joback Method
tc	1159.80	K	Joback Method
tf	563.41	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.35	J/mol×K	943.32	Joback Method
cpg	914.27	J/mol×K	979.40	Joback Method
cpg	925.98	J/mol×K	1015.48	Joback Method
cpg	936.51	J/mol×K	1051.56	Joback Method
cpg	945.88	J/mol×K	1087.64	Joback Method
cpg	954.13	J/mol×K	1123.72	Joback Method
cpg	961.27	J/mol×K	1159.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354440&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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