Sebacic acid, 4-cyanophenyl octyl ester

Inchi: InChI=1S/C25H37NO4/c1-2-3-4-5-10-13-20-29-24(27)14-11-8-6-7-9-12-15-25(28)30-23-
InchiKey: DZBWCGXTPBPOHC-UHFFFAOYSA-N
Formula: C25H37NO4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 415.57

Physical Properties

Property code	Value	Unit	Source
gf	-72.26	kJ/mol	Joback Method
hf	-658.99	kJ/mol	Joback Method
hfus	61.24	kJ/mol	Joback Method
hvap	102.97	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	6.488		Crippen Method
mcvol	355.610	ml/mol	McGowan Method
pc	955.55	kPa	Joback Method
rinpol	3319.00		NIST Webbook
rinpol	3319.00		NIST Webbook
tb	1057.72	K	Joback Method
tc	1296.97	K	Joback Method
tf	619.76	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1202.16	J/mol×K	1057.72	Joback Method
cpg	1216.07	J/mol×K	1097.59	Joback Method
cpg	1228.38	J/mol×K	1137.47	Joback Method
cpg	1239.12	J/mol×K	1177.34	Joback Method
cpg	1248.38	J/mol×K	1217.22	Joback Method
cpg	1256.20	J/mol×K	1257.09	Joback Method
cpg	1262.64	J/mol×K	1296.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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