

Sebacic acid, 4-cyanophenyl hexyl ester

Inchi: InChI=1S/C23H33NO4/c1-2-3-4-11-18-27-22(25)12-9-7-5-6-8-10-13-23(26)28-21-16-14-
InchiKey: WVXMOLAKOIAAYIE-UHFFFAOYSA-N
Formula: C23H33NO4
SMILES: CCCCCCOC(=O)CCCCCCCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 387.51

Physical Properties

Property code	Value	Unit	Source
gf	-89.10	kJ/mol	Joback Method
hf	-617.71	kJ/mol	Joback Method
hfus	56.06	kJ/mol	Joback Method
hvap	98.52	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.708		Crippen Method
mvol	327.430	ml/mol	McGowan Method
pc	1079.93	kPa	Joback Method
rinpol	3108.00		NIST Webbook
rinpol	3108.00		NIST Webbook
tb	1011.96	K	Joback Method
tc	1238.93	K	Joback Method
tf	597.22	K	Joback Method
vc	1.290	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1080.44	J/molxK	1011.96	Joback Method
cpg	1093.93	J/molxK	1049.79	Joback Method
cpg	1106.00	J/molxK	1087.62	Joback Method
cpg	1116.70	J/molxK	1125.44	Joback Method
cpg	1126.07	J/molxK	1163.27	Joback Method
cpg	1134.14	J/molxK	1201.10	Joback Method
cpg	1140.97	J/molxK	1238.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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