

Sebacic acid, 3-nitrophenyl nonyl ester

Inchi:	InChI=1S/C25H39NO6/c1-2-3-4-5-8-11-14-20-31-24(27)18-12-9-6-7-10-13-19-25(28)32-
InchiKey:	SXMYOYIKYJIJEF-UHFFFAOYSA-N
Formula:	C25H39NO6
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	449.58

Physical Properties

Property code	Value	Unit	Source
gf	-169.89	kJ/mol	Joback Method
hf	-834.63	kJ/mol	Joback Method
hfus	71.09	kJ/mol	Joback Method
hvap	109.08	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	6.915		Crippen Method
mvol	371.650	ml/mol	McGowan Method
pc	977.78	kPa	Joback Method
rinpol	3528.00		NIST Webbook
rinpol	3528.00		NIST Webbook
tb	1107.48	K	Joback Method
tc	1359.81	K	Joback Method
tf	698.38	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.28	J/mol×K	1107.48	Joback Method
cpg	1304.53	J/mol×K	1149.54	Joback Method
cpg	1316.00	J/mol×K	1191.59	Joback Method
cpg	1325.78	J/mol×K	1233.65	Joback Method
cpg	1333.94	J/mol×K	1275.70	Joback Method
cpg	1340.56	J/mol×K	1317.76	Joback Method
cpg	1345.73	J/mol×K	1359.81	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=U354921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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