Sebacic acid, 2-(3-nitrophenyl)ethyl propyl ester

Inchi: InChI=1S/C21H31NO6/c1-2-15-27-20(23)12-7-5-3-4-6-8-13-21(24)28-16-14-18-10-9-11-
InchiKey: ODMWTVKKTOCWPD-UHFFFAOYSA-N
Formula: C21H31NO6
SMILES: CCCOC(=O)CCCCCCCCC(=O)OCCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 393.47

Physical Properties

Property code	Value	Unit	Source
gf	-203.57	kJ/mol	Joback Method
hf	-752.07	kJ/mol	Joback Method
hfus	60.73	kJ/mol	Joback Method
hvap	100.18	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.755		Crippen Method
mcvol	315.290	ml/mol	McGowan Method
pc	1262.85	kPa	Joback Method
rinpol	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook
tb	1015.96	K	Joback Method
tc	1244.92	K	Joback Method
tf	653.30	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.19	J/mol×K	1015.96	Joback Method
cpg	1060.90	J/mol×K	1054.12	Joback Method
cpg	1072.19	J/mol×K	1092.28	Joback Method
cpg	1082.12	J/mol×K	1130.44	Joback Method
cpg	1090.71	J/mol×K	1168.60	Joback Method
cpg	1098.02	J/mol×K	1206.76	Joback Method
cpg	1104.09	J/mol×K	1244.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380655&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