Sebacic acid, isobutyl 3-nitrophenyl ester

Inchi: InChI=1S/C20H29NO6/c1-16(2)15-26-19(22)12-7-5-3-4-6-8-13-20(23)27-18-11-9-10-17(
InchiKey: OROMGPQQXKVYFZ-UHFFFAOYSA-N
Formula: C20H29NO6
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 379.45

Physical Properties

Property code	Value	Unit	Source
gf	-214.43	kJ/mol	Joback Method
hf	-736.71	kJ/mol	Joback Method
hfus	54.62	kJ/mol	Joback Method
hvap	97.57	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.820		Crippen Method
mcvol	301.200	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
rinpol	2944.00		NIST Webbook
tb	992.64	K	Joback Method
tc	1219.48	K	Joback Method
tf	627.03	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.83	J/mol×K	992.64	Joback Method
cpg	1001.42	J/mol×K	1030.45	Joback Method
cpg	1012.62	J/mol×K	1068.25	Joback Method
cpg	1022.49	J/mol×K	1106.06	Joback Method
cpg	1031.05	J/mol×K	1143.87	Joback Method
cpg	1038.35	J/mol×K	1181.67	Joback Method
cpg	1044.43	J/mol×K	1219.48	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=U354914&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