Sebacic acid, ethyl 3-methyl-2-nitrobenzyl ester

Inchi: InChI=1S/C20H29NO6/c1-3-26-18(22)13-8-6-4-5-7-9-14-19(23)27-15-17-12-10-11-16(2)

InchiKey: AYXMUETXQZUDQF-UHFFFAOYSA-N

Formula: C20H29NO6

SMILES: CCOC(=O)CCCCCCCCC(=O)OCc1cccc(C)c1[N+](=O)[O-]

Mol. weight [g/mol]: 379.45

Physical Properties

Property code	Value	Unit	Source
gf	-221.62	kJ/mol	Joback Method
hf	-742.90	kJ/mol	Joback Method
hfus	57.75	kJ/mol	Joback Method
hvap	98.62	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.630		Crippen Method
mcvol	301.200	ml/mol	McGowan Method
pc	1338.82	kPa	Joback Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
tb	998.06	K	Joback Method
tc	1224.88	K	Joback Method
tf	654.55	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.14	J/mol×K	998.06	Joback Method
cpg	999.59	J/mol×K	1035.86	Joback Method
cpg	1010.65	J/mol×K	1073.67	Joback Method
cpg	1020.35	J/mol×K	1111.47	Joback Method
cpg	1028.73	J/mol×K	1149.27	Joback Method
cpg	1035.80	J/mol×K	1187.07	Joback Method
cpg	1041.61	J/mol×K	1224.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380729&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

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