Sebacic acid, 3-nitro-4-chlorobenzyl propyl ester

Inchi: InChI=1S/C20H28ClNO6/c1-2-13-27-19(23)9-7-5-3-4-6-8-10-20(24)28-15-16-11-12-17(2

InchiKey: WNKSREHRIMTQPK-UHFFFAOYSA-N

Formula: C20H28ClNO6

SMILES: CCCOC(=O)CCCCCCCCC(=O)OCc1ccc(Cl)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 413.89

Physical Properties

Property code	Value	Unit	Source
gf	-233.55	kJ/mol	Joback Method
hf	-758.64	kJ/mol	Joback Method
hfus	61.95	kJ/mol	Joback Method
hvap	103.00	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.365		Crippen Method
mcvol	313.440	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook
tb	1035.49	K	Joback Method
tc	1269.05	K	Joback Method
tf	684.47	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1007.50	J/mol×K	1035.49	Joback Method
cpg	1018.65	J/mol×K	1074.42	Joback Method
cpg	1028.37	J/mol×K	1113.34	Joback Method
cpg	1036.72	J/mol×K	1152.27	Joback Method
cpg	1043.73	J/mol×K	1191.20	Joback Method
cpg	1049.44	J/mol×K	1230.13	Joback Method
cpg	1053.87	J/mol×K	1269.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380580&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