Succinic acid, cyclohexylmethyl 3-nitrophenyl ester

Inchi: InChI=1S/C17H21NO6/c19-16(23-12-13-5-2-1-3-6-13)9-10-17(20)24-15-8-4-7-14(11-15)
InchiKey: QXUVHPJAWWEFDF-UHFFFAOYSA-N
Formula: C17H21NO6
SMILES: O=C(CCC(=O)Oc1cccc([N+](=O)[O-])c1)OCC1CCCCC1
Mol. weight [g/mol]: 335.35

Physical Properties

Property code	Value	Unit	Source
gf	-212.80	kJ/mol	Joback Method
hf	-615.19	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	91.71	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.404		Crippen Method
mcvol	248.070	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
tb	943.99	K	Joback Method
tc	1187.95	K	Joback Method
tf	615.60	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.53	J/mol×K	943.99	Joback Method
cpg	816.90	J/mol×K	984.65	Joback Method
cpg	827.66	J/mol×K	1025.31	Joback Method
cpg	836.84	J/mol×K	1065.97	Joback Method
cpg	844.48	J/mol×K	1106.63	Joback Method
cpg	850.61	J/mol×K	1147.29	Joback Method
cpg	855.28	J/mol×K	1187.95	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=U390139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume