Succinic acid, 2-ethylhexyl 3-nitrophenyl ester

Inchi: InChI=1S/C18H25NO6/c1-3-5-7-14(4-2)13-24-17(20)10-11-18(21)25-16-9-6-8-15(12-16)
InchiKey: HRDDXGLXDDNKNI-UHFFFAOYSA-N
Formula: C18H25NO6
SMILES: CCCCC(CC)COC(=O)CCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 351.39

Physical Properties

Property code	Value	Unit	Source
gf	-231.27	kJ/mol	Joback Method
hf	-695.43	kJ/mol	Joback Method
hfus	49.44	kJ/mol	Joback Method
hvap	93.11	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.040		Crippen Method
mcvol	273.020	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	2646.00		NIST Webbook
rinpol	2646.00		NIST Webbook
tb	946.88	K	Joback Method
tc	1171.09	K	Joback Method
tf	604.49	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.95	J/mol×K	946.88	Joback Method
cpg	883.36	J/mol×K	984.25	Joback Method
cpg	894.49	J/mol×K	1021.62	Joback Method
cpg	904.36	J/mol×K	1058.99	Joback Method
cpg	913.01	J/mol×K	1096.36	Joback Method
cpg	920.45	J/mol×K	1133.72	Joback Method
cpg	926.74	J/mol×K	1171.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390138&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

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