Succinic acid, 2-(4-nitrophenoxy)ethyl propyl ester

Inchi: InChI=1S/C15H19NO7/c1-2-9-22-14(17)7-8-15(18)23-11-10-21-13-5-3-12(4-6-13)16(19)
InchiKey: JELGRMPWJAZIJA-UHFFFAOYSA-N
Formula: C15H19NO7
SMILES: CCCOC(=O)CCC(=O)OCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 325.31

Physical Properties

Property code	Value	Unit	Source
gf	-359.09	kJ/mol	Joback Method
hf	-760.45	kJ/mol	Joback Method
hfus	46.38	kJ/mol	Joback Method
hvap	89.23	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.250		Crippen Method
mcvol	236.620	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	2571.00		NIST Webbook
rinpol	2571.00		NIST Webbook
tb	901.10	K	Joback Method
tc	1124.19	K	Joback Method
tf	607.91	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.14	J/mol×K	901.10	Joback Method
cpg	735.42	J/mol×K	938.28	Joback Method
cpg	745.45	J/mol×K	975.46	Joback Method
cpg	754.25	J/mol×K	1012.65	Joback Method
cpg	761.80	J/mol×K	1049.83	Joback Method
cpg	768.11	J/mol×K	1087.01	Joback Method
cpg	773.19	J/mol×K	1124.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381133&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