Succinic acid, isobutyl 2-nitrophenethyl ester

Inchi: InChI=1S/C16H21NO6/c1-12(2)11-23-16(19)8-7-15(18)22-10-9-13-5-3-4-6-14(13)17(20)
InchiKey: BEGNAIARYNZYBM-UHFFFAOYSA-N
Formula: C16H21NO6
SMILES: CC(C)COC(=O)CCC(=O)OCCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 323.34

Physical Properties

Property code	Value	Unit	Source
gf	-248.11	kJ/mol	Joback Method
hf	-654.15	kJ/mol	Joback Method
hfus	44.26	kJ/mol	Joback Method
hvap	88.66	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.660		Crippen Method
mcvol	244.840	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook
tb	901.12	K	Joback Method
tc	1126.06	K	Joback Method
tf	581.95	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.49	J/mol×K	901.12	Joback Method
cpg	767.68	J/mol×K	938.61	Joback Method
cpg	778.65	J/mol×K	976.10	Joback Method
cpg	788.44	J/mol×K	1013.59	Joback Method
cpg	797.05	J/mol×K	1051.08	Joback Method
cpg	804.52	J/mol×K	1088.57	Joback Method
cpg	810.87	J/mol×K	1126.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381269&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