Succinic acid, 3-methylbut-2-yl 3-nitrophenyl ester

Inchi: InChI=1S/C15H19NO6/c1-10(2)11(3)21-14(17)7-8-15(18)22-13-6-4-5-12(9-13)16(19)20/
InchiKey: DVBBXHNIOZBFNH-UHFFFAOYSA-N
Formula: C15H19NO6
SMILES: CC(C)C(C)OC(=O)CCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 309.31

Physical Properties

Property code	Value	Unit	Source
gf	-258.97	kJ/mol	Joback Method
hf	-638.79	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	86.05	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	2.868		Crippen Method
mcvol	230.750	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		NIST Webbook
tb	877.80	K	Joback Method
tc	1107.20	K	Joback Method
tf	555.68	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.38	J/mol×K	877.80	Joback Method
cpg	711.54	J/mol×K	916.03	Joback Method
cpg	722.47	J/mol×K	954.27	Joback Method
cpg	732.20	J/mol×K	992.50	Joback Method
cpg	740.74	J/mol×K	1030.73	Joback Method
cpg	748.12	J/mol×K	1068.96	Joback Method
cpg	754.35	J/mol×K	1107.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390134&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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