Succinic acid, 4-methyl-3-nitrobenzyl propyl ester

Inchi: InChI=1S/C15H19NO6/c1-3-8-21-14(17)6-7-15(18)22-10-12-5-4-11(2)13(9-12)16(19)20/l

InchiKey: YCRZNMBSOWMHFT-UHFFFAOYSA-N

Formula: C15H19NO6

SMILES: CCCOC(=O)CCC(=O)OCc1ccc(C)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 309.31

Physical Properties

Property code	Value	Unit	Source
gf	-263.72	kJ/mol	Joback Method
hf	-639.70	kJ/mol	Joback Method
hfus	44.80	kJ/mol	Joback Method
hvap	87.49	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.680		Crippen Method
mcvol	230.750	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook
tb	883.66	K	Joback Method
tc	1108.06	K	Joback Method
tf	598.20	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.82	J/mol×K	883.66	Joback Method
cpg	708.65	J/mol×K	921.06	Joback Method
cpg	719.33	J/mol×K	958.46	Joback Method
cpg	728.87	J/mol×K	995.86	Joback Method
cpg	737.28	J/mol×K	1033.26	Joback Method
cpg	744.57	J/mol×K	1070.66	Joback Method
cpg	750.76	J/mol×K	1108.06	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=U381127&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