Succinic acid, 3,4-dimethylphenyl N,N-diethyl-2-aminoethyl ester

Inchi: InChI=1S/C18H27NO4/c1-5-19(6-2)11-12-22-17(20)9-10-18(21)23-16-8-7-14(3)15(4)13-

InchiKey: JLGLHKDJMKEMRY-UHFFFAOYSA-N

Formula: C18H27NO4

SMILES: CCN(CC)CCOC(=O)CCC(=O)Oc1ccc(C)c(C)c1

Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
gf	-163.23	kJ/mol	Joback Method
hf	-623.33	kJ/mol	Joback Method
hfus	44.23	kJ/mol	Joback Method
hvap	79.62	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.874		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	812.90	K	Joback Method
tc	1012.69	K	Joback Method
tf	520.87	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.18	J/mol×K	812.90	Joback Method
cpg	817.81	J/mol×K	846.20	Joback Method
cpg	832.36	J/mol×K	879.50	Joback Method
cpg	845.87	J/mol×K	912.79	Joback Method
cpg	858.35	J/mol×K	946.09	Joback Method
cpg	869.82	J/mol×K	979.39	Joback Method
cpg	880.30	J/mol×K	1012.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357570&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