Succinic acid, phenethyl N,N-diethyl-2-aminoethyl ester

Inchi: InChI=1S/C18H27NO4/c1-3-19(4-2)13-15-23-18(21)11-10-17(20)22-14-12-16-8-6-5-7-9-
InchiKey: YIBFVKFMZGCTJO-UHFFFAOYSA-N
Formula: C18H27NO4
SMILES: CCN(CC)CCOC(=O)CCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
gf	-143.97	kJ/mol	Joback Method
hf	-600.39	kJ/mol	Joback Method
hfus	45.01	kJ/mol	Joback Method
hvap	78.29	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.438		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2384.00		NIST Webbook
tb	802.94	K	Joback Method
tc	1001.06	K	Joback Method
tf	495.83	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.56	J/mol×K	802.94	Joback Method
cpg	819.36	J/mol×K	835.96	Joback Method
cpg	834.09	J/mol×K	868.98	Joback Method
cpg	847.77	J/mol×K	902.00	Joback Method
cpg	860.43	J/mol×K	935.02	Joback Method
cpg	872.11	J/mol×K	968.04	Joback Method
cpg	882.84	J/mol×K	1001.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358009&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