Succinic acid, 4-isopropylphenyl N,N-diethyl-2-aminoethyl ester

Inchi: InChI=1S/C19H29NO4/c1-5-20(6-2)13-14-23-18(21)11-12-19(22)24-17-9-7-16(8-10-17)1

InchiKey: RHTWOGDNMJMBNT-UHFFFAOYSA-N

Formula: C19H29NO4

SMILES: CCN(CC)CCOC(=O)CCC(=O)Oc1ccc(C(C)C)cc1

Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
gf	-147.62	kJ/mol	Joback Method
hf	-637.78	kJ/mol	Joback Method
hfus	43.69	kJ/mol	Joback Method
hvap	80.79	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.381		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	2421.00		NIST Webbook
tb	830.36	K	Joback Method
tc	1031.43	K	Joback Method
tf	504.62	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.65	J/mol×K	830.36	Joback Method
cpg	877.73	J/mol×K	863.87	Joback Method
cpg	892.66	J/mol×K	897.38	Joback Method
cpg	906.48	J/mol×K	930.90	Joback Method
cpg	919.22	J/mol×K	964.41	Joback Method
cpg	930.90	J/mol×K	997.92	Joback Method
cpg	941.56	J/mol×K	1031.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360724&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

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