

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

Inchi:	InChI=1S/C19H29NO5/c1-5-20(6-2)13-14-23-18(21)11-12-19(22)25-17-10-8-7-9-16(17)2
InchiKey:	AXSOXVDZJQIAJE-UHFFFAOYSA-N
Formula:	C19H29NO5
SMILES:	CCN(CC)CCOC(=O)CCC(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]:	351.44

Physical Properties

Property code	Value	Unit	Source
gf	-252.62	kJ/mol	Joback Method
hf	-770.00	kJ/mol	Joback Method
hfus	44.88	kJ/mol	Joback Method
hvap	83.20	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.044		Crippen Method
mcvol	285.540	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	2435.00		NIST Webbook
tb	852.78	K	Joback Method
tc	1054.88	K	Joback Method
tf	526.85	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.88	J/molxK	852.78	Joback Method
cpg	906.44	J/molxK	886.46	Joback Method
cpg	920.80	J/molxK	920.15	Joback Method
cpg	933.96	J/molxK	953.83	Joback Method
cpg	945.95	J/molxK	987.51	Joback Method
cpg	956.77	J/molxK	1021.20	Joback Method
cpg	966.45	J/molxK	1054.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U357978&Units=SI

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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