Succinic acid, 3,4-dimethylphenyl 2-(dimethylamino)ethyl ester

Inchi: InChI=1S/C16H23NO4/c1-12-5-6-14(11-13(12)2)21-16(19)8-7-15(18)20-10-9-17(3)4/h5-

InchiKey: WGPXHQBLDRNMPL-UHFFFAOYSA-N

Formula: C16H23NO4

SMILES: Cc1ccc(OC(=O)CCC(=O)OCCN(C)C)cc1C

Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
gf	-180.07	kJ/mol	Joback Method
hf	-582.05	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	75.16	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.094		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2264.00		NIST Webbook
rinpol	2264.00		NIST Webbook
tb	767.14	K	Joback Method
tc	968.23	K	Joback Method
tf	498.33	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.28	J/mol×K	767.14	Joback Method
cpg	703.39	J/mol×K	800.65	Joback Method
cpg	717.51	J/mol×K	834.17	Joback Method
cpg	730.64	J/mol×K	867.68	Joback Method
cpg	742.82	J/mol×K	901.20	Joback Method
cpg	754.04	J/mol×K	934.71	Joback Method
cpg	764.34	J/mol×K	968.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357564&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
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