Succinic acid, 2-methylphenyl 2-(dimethylamino)ethyl ester

Inchi: InChI=1S/C15H21NO4/c1-12-6-4-5-7-13(12)20-15(18)9-8-14(17)19-11-10-16(2)3/h4-7H,

InchiKey: PBAVUQWUHBGALI-UHFFFAOYSA-N

Formula: C15H21NO4

SMILES: Cc1ccccc1OC(=O)CCC(=O)OCCN(C)C

Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
gf	-178.86	kJ/mol	Joback Method
hf	-549.94	kJ/mol	Joback Method
hfus	36.85	kJ/mol	Joback Method
hvap	72.28	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.785		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook
tb	739.28	K	Joback Method
tc	941.06	K	Joback Method
tf	474.54	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.65	J/mol×K	739.28	Joback Method
cpg	648.56	J/mol×K	772.91	Joback Method
cpg	662.50	J/mol×K	806.54	Joback Method
cpg	675.48	J/mol×K	840.17	Joback Method
cpg	687.53	J/mol×K	873.80	Joback Method
cpg	698.66	J/mol×K	907.43	Joback Method
cpg	708.89	J/mol×K	941.06	Joback Method

Sources

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=U357536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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