Succinic acid, 3-methylbut-2-en-1-yl 3-methoxyphenyl ester

Inchi: InChI=1S/C16H20O5/c1-12(2)9-10-20-15(17)7-8-16(18)21-14-6-4-5-13(11-14)19-3/h4-6,

InchiKey: GWVVYEBKTHTTMW-UHFFFAOYSA-N

Formula: C16H20O5

SMILES: COc1cccc(OC(=O)CCC(=O)OCC=C(C)C)c1

Mol. weight [g/mol]: 292.33

Physical Properties

Property code	Value	Unit	Source
gf	-314.55	kJ/mol	Joback Method
hf	-662.90	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Joback Method
hvap	74.91	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.890		Crippen Method
mcvol	228.990	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook
tb	776.18	K	Joback Method
tc	985.59	K	Joback Method
tf	456.53	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.85	J/mol×K	776.18	Joback Method
cpg	665.23	J/mol×K	811.08	Joback Method
cpg	678.61	J/mol×K	845.98	Joback Method
cpg	690.98	J/mol×K	880.88	Joback Method
cpg	702.38	J/mol×K	915.78	Joback Method
cpg	712.81	J/mol×K	950.69	Joback Method
cpg	722.27	J/mol×K	985.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390978&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