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

Inchi: InChI=1S/C17H22O4/c1-12(2)10-11-20-16(18)8-9-17(19)21-15-7-5-6-13(3)14(15)4/h5-7,

InchiKey: PYTPFZOTHJFKTG-UHFFFAOYSA-N

Formula: C17H22O4

SMILES: CC(C)=CCOC(=O)CCC(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-210.76	kJ/mol	Joback Method
hf	-562.79	kJ/mol	Joback Method
hfus	37.52	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.498		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	781.62	K	Joback Method
tc	991.04	K	Joback Method
tf	458.09	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.08	J/mol×K	781.62	Joback Method
cpg	693.06	J/mol×K	816.52	Joback Method
cpg	707.04	J/mol×K	851.43	Joback Method
cpg	720.05	J/mol×K	886.33	Joback Method
cpg	732.11	J/mol×K	921.24	Joback Method
cpg	743.24	J/mol×K	956.14	Joback Method
cpg	753.47	J/mol×K	991.04	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=U390018&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