Succinic acid, di(2,3-dimethylphenyl) ester

Inchi: InChI=1S/C20H22O4/c1-13-7-5-9-17(15(13)3)23-19(21)11-12-20(22)24-18-10-6-8-14(2)1
InchiKey: NLNCMIOEWJKLSV-UHFFFAOYSA-N
Formula: C20H22O4
SMILES: Cc1cccc(OC(=O)CCC(=O)Oc2cccc(C)c2C)c1C
Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-164.02	kJ/mol	Joback Method
hf	-518.55	kJ/mol	Joback Method
hfus	39.66	kJ/mol	Joback Method
hvap	85.63	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.211		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2614.00		NIST Webbook
tb	882.86	K	Joback Method
tc	1108.90	K	Joback Method
tf	562.40	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.05	J/mol×K	882.86	Joback Method
cpg	834.60	J/mol×K	1071.23	Joback Method
cpg	825.84	J/mol×K	1033.56	Joback Method
cpg	815.81	J/mol×K	995.88	Joback Method
cpg	804.52	J/mol×K	958.21	Joback Method
cpg	791.94	J/mol×K	920.53	Joback Method
cpg	842.13	J/mol×K	1108.90	Joback Method
dvisc	0.0000590	Pa×s	882.86	Joback Method
dvisc	0.0000724	Pa×s	829.45	Joback Method

dvisc	0.0000912	Pa×s	776.04	Joback Method
dvisc	0.0001190	Pa×s	722.63	Joback Method
dvisc	0.0001620	Pa×s	669.22	Joback Method
dvisc	0.0002326	Pa×s	615.81	Joback Method
dvisc	0.0003578	Pa×s	562.40	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=U349634&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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