Succinic acid, cyclohexylmethyl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C19H26O4/c1-14-7-6-10-17(15(14)2)23-19(21)12-11-18(20)22-13-16-8-4-3-5-9

InchiKey: IRCNTFJRJMCDQY-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: Cc1cccc(OC(=O)CCC(=O)OCC2CCCCC2)c1C

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-241.14	kJ/mol	Joback Method
hf	-657.18	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	80.23	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.113		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook
tb	842.89	K	Joback Method
tc	1064.59	K	Joback Method
tf	507.05	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.28	J/mol×K	842.89	Joback Method
cpg	883.28	J/mol×K	1027.64	Joback Method
cpg	872.12	J/mol×K	990.69	Joback Method
cpg	859.57	J/mol×K	953.74	Joback Method
cpg	845.59	J/mol×K	916.79	Joback Method
cpg	830.17	J/mol×K	879.84	Joback Method
cpg	893.05	J/mol×K	1064.59	Joback Method
dvisc	0.0000661	Pa×s	842.89	Joback Method

dvisc	0.0000843	Pa×s	786.92	Joback Method
dvisc	0.0001118	Pa×s	730.94	Joback Method
dvisc	0.0001551	Pa×s	674.97	Joback Method
dvisc	0.0002285	Pa×s	619.00	Joback Method
dvisc	0.0003636	Pa×s	563.02	Joback Method
dvisc	0.0006409	Pa×s	507.05	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=U390024&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