Succinic acid, cyclohexylmethyl 2-methoxy-5-methylphenyl ester

Inchi: InChI=1S/C19H26O5/c1-14-8-9-16(22-2)17(12-14)24-19(21)11-10-18(20)23-13-15-6-4-3

InchiKey: VJAGGLKAAYAABN-UHFFFAOYSA-N

Formula: C19H26O5

SMILES: COc1ccc(C)cc1OC(=O)CCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 334.41

Physical Properties

Property code	Value	Unit	Source
gf	-346.14	kJ/mol	Joback Method
hf	-789.40	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	82.64	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.813		Crippen Method
mcvol	264.700	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	2577.00		NIST Webbook
tb	865.31	K	Joback Method
tc	1086.00	K	Joback Method
tf	529.28	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.13	J/mol×K	865.31	Joback Method
cpg	858.22	J/mol×K	902.09	Joback Method
cpg	872.77	J/mol×K	938.87	Joback Method
cpg	885.79	J/mol×K	975.66	Joback Method
cpg	897.28	J/mol×K	1012.44	Joback Method
cpg	907.24	J/mol×K	1049.22	Joback Method
cpg	915.68	J/mol×K	1086.00	Joback Method
dvisc	0.0004535	Pa×s	529.28	Joback Method
dvisc	0.0002630	Pa×s	585.28	Joback Method

dvisc	0.0001678	Pa×s	641.29	Joback Method
dvisc	0.0001150	Pa×s	697.29	Joback Method
dvisc	0.0000834	Pa×s	753.30	Joback Method
dvisc	0.0000633	Pa×s	809.30	Joback Method
dvisc	0.0000497	Pa×s	865.31	Joback Method

Sources

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=U390962&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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