Succinic acid, cyclohexylmethyl 2-methoxyphenyl ester

Inchi: InChI=1S/C18H24O5/c1-21-15-9-5-6-10-16(15)23-18(20)12-11-17(19)22-13-14-7-3-2-4-8

InchiKey: PXTPOYDFTZNLIV-UHFFFAOYSA-N

Formula: C18H24O5

SMILES: COc1ccccc1OC(=O)CCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 320.38

Physical Properties

Property code	Value	Unit	Source
gf	-344.93	kJ/mol	Joback Method
hf	-757.29	kJ/mol	Joback Method
hfus	34.62	kJ/mol	Joback Method
hvap	79.75	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.504		Crippen Method
mcvol	250.610	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpol	2485.00		NIST Webbook
rinpol	2485.00		NIST Webbook
tb	837.45	K	Joback Method
tc	1059.18	K	Joback Method
tf	505.49	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.54	J/mol×K	837.45	Joback Method
cpg	800.83	J/mol×K	874.40	Joback Method
cpg	815.61	J/mol×K	911.36	Joback Method
cpg	828.91	J/mol×K	948.31	Joback Method
cpg	840.72	J/mol×K	985.27	Joback Method
cpg	851.05	J/mol×K	1022.22	Joback Method
cpg	859.93	J/mol×K	1059.18	Joback Method
dvisc	0.0005796	Pa×s	505.49	Joback Method

dvisc	0.0003246	Pa×s	560.82	Joback Method
dvisc	0.0002017	Pa×s	616.14	Joback Method
dvisc	0.0001356	Pa×s	671.47	Joback Method
dvisc	0.0000968	Pa×s	726.80	Joback Method
dvisc	0.0000725	Pa×s	782.12	Joback Method
dvisc	0.0000564	Pa×s	837.45	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=U389711&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