Succinic acid, 2-ethylhexyl trans-4-methylcyclohexyl ester

Inchi: InChI=1S/C19H34O4/c1-4-6-7-16(5-2)14-22-18(20)12-13-19(21)23-17-10-8-15(3)9-11-17

InchiKey: UIYMXSXRLVWZMC-UHFFFAOYSA-N

Formula: C19H34O4

SMILES: CCCCC(CC)COC(=O)CCC(=O)OC1CCC(C)CC1

Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-344.44	kJ/mol	Joback Method
hf	-896.39	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	75.93	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.648		Crippen Method
mcvol	282.590	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	2276.00		NIST Webbook
rinpol	2276.00		NIST Webbook
tb	801.14	K	Joback Method
tc	997.68	K	Joback Method
tf	436.35	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.24	J/mol×K	801.14	Joback Method
cpg	928.59	J/mol×K	833.90	Joback Method
cpg	946.62	J/mol×K	866.65	Joback Method
cpg	963.37	J/mol×K	899.41	Joback Method
cpg	978.84	J/mol×K	932.17	Joback Method
cpg	993.04	J/mol×K	964.93	Joback Method
cpg	1006.00	J/mol×K	997.68	Joback Method
dvisc	0.0013131	Pa×s	436.35	Joback Method

dvisc	0.0006075	Pa×s	497.15	Joback Method
dvisc	0.0003324	Pa×s	557.95	Joback Method
dvisc	0.0002048	Pa×s	618.75	Joback Method
dvisc	0.0001376	Pa×s	679.54	Joback Method
dvisc	0.0000987	Pa×s	740.34	Joback Method
dvisc	0.0000744	Pa×s	801.14	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=U390071&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