Succinic acid, cyclohexylmethyl 1-phenylpropyl ester

Inchi: InChI=1S/C20H28O4/c1-2-18(17-11-7-4-8-12-17)24-20(22)14-13-19(21)23-15-16-9-5-3-6

InchiKey: AYEAZUYCUDKKBD-UHFFFAOYSA-N

Formula: C20H28O4

SMILES: CCC(OC(=O)CCC(=O)OCC1CCCCC1)c1ccccc1

Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-215.90	kJ/mol	Joback Method
hf	-660.16	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	80.74	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.585		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	2393.00		NIST Webbook
rinpol	2393.00		NIST Webbook
tb	855.37	K	Joback Method
tc	1076.59	K	Joback Method
tf	478.28	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.10	J/mol×K	855.37	Joback Method
cpg	891.38	J/mol×K	892.24	Joback Method
cpg	907.13	J/mol×K	929.11	Joback Method
cpg	921.40	J/mol×K	965.98	Joback Method
cpg	934.21	J/mol×K	1002.85	Joback Method
cpg	945.62	J/mol×K	1039.72	Joback Method
cpg	955.66	J/mol×K	1076.59	Joback Method
dvisc	0.0009144	Pa×s	478.28	Joback Method

dvisc	0.0004281	Pa×s	541.13	Joback Method
dvisc	0.0002347	Pa×s	603.98	Joback Method
dvisc	0.0001441	Pa×s	666.83	Joback Method
dvisc	0.0000962	Pa×s	729.67	Joback Method
dvisc	0.0000685	Pa×s	792.52	Joback Method
dvisc	0.0000513	Pa×s	855.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389931&Units=SI
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

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