Succinic acid, cyclohexylmethyl 3-phenylpropyl ester

Inchi: InChI=1S/C20H28O4/c21-19(23-15-7-12-17-8-3-1-4-9-17)13-14-20(22)24-16-18-10-5-2-6-11-18/h1,3-4,8-9,18H,2,5-7,10-16H2

InchiKey: HDWCSQGQABBUTI-UHFFFAOYSA-N

Formula: C20H28O4

SMILES: O=C(CCC(=O)OCC1CCCCC1)OCCCc1ccccc1

Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-213.46	kJ/mol	Joback Method
hf	-654.88	kJ/mol	Joback Method
hfus	39.01	kJ/mol	Joback Method
hvap	81.13	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.066		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	2623.00		NIST Webbook
rinpol	2623.00		NIST Webbook
tb	855.81	K	Joback Method
tc	1074.27	K	Joback Method
tf	493.28	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.59	J/mol×K	855.81	Joback Method
cpg	890.67	J/mol×K	892.22	Joback Method
cpg	906.28	J/mol×K	928.63	Joback Method
cpg	920.45	J/mol×K	965.04	Joback Method
cpg	933.22	J/mol×K	1001.45	Joback Method
cpg	944.62	J/mol×K	1037.86	Joback Method
cpg	954.71	J/mol×K	1074.27	Joback Method
dvisc	0.0007938	Pa×s	493.28	Joback Method

dvisc	0.0004009	Pa×s	553.70	Joback Method
dvisc	0.0002316	Pa×s	614.12	Joback Method
dvisc	0.0001476	Pa×s	674.54	Joback Method
dvisc	0.0001013	Pa×s	734.97	Joback Method
dvisc	0.0000736	Pa×s	795.39	Joback Method
dvisc	0.0000560	Pa×s	855.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389730&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