Succinic acid, cyclohexylmethyl phenethyl ester

Inchi: InChI=1S/C19H26O4/c20-18(22-14-13-16-7-3-1-4-8-16)11-12-19(21)23-15-17-9-5-2-6-10

InchiKey: VPAOUODPXPXCKS-UHFFFAOYSA-N

Formula: C19H26O4

SMILES: O=C(CCC(=O)OCC1CCCCC1)OCCc1ccccc1

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-221.88	kJ/mol	Joback Method
hf	-634.24	kJ/mol	Joback Method
hfus	36.42	kJ/mol	Joback Method
hvap	78.91	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.676		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2493.00		NIST Webbook
tb	832.93	K	Joback Method
tc	1053.12	K	Joback Method
tf	482.01	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.72	J/mol×K	832.93	Joback Method
cpg	831.86	J/mol×K	869.63	Joback Method
cpg	847.53	J/mol×K	906.33	Joback Method
cpg	861.77	J/mol×K	943.02	Joback Method
cpg	874.63	J/mol×K	979.72	Joback Method
cpg	886.12	J/mol×K	1016.42	Joback Method
cpg	896.30	J/mol×K	1053.12	Joback Method
dvisc	0.0008834	Pa×s	482.01	Joback Method
dvisc	0.0004511	Pa×s	540.50	Joback Method

dvisc	0.0002627	Pa×s	598.98	Joback Method
dvisc	0.0001684	Pa×s	657.47	Joback Method
dvisc	0.0001161	Pa×s	715.96	Joback Method
dvisc	0.0000846	Pa×s	774.44	Joback Method
dvisc	0.0000645	Pa×s	832.93	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=U389749&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