Succinic acid, cyclohexylmethyl 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C17H30O4/c1-13(17(2,3)4)21-16(19)11-10-15(18)20-12-14-8-6-5-7-9-14/h13-1

InchiKey: NCFVALNQQFIYMH-UHFFFAOYSA-N

Formula: C17H30O4

SMILES: CC(OC(=O)CCC(=O)OCC1CCCCC1)C(C)(C)C

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-350.73	kJ/mol	Joback Method
hf	-843.52	kJ/mol	Joback Method
hfus	26.26	kJ/mol	Joback Method
hvap	70.49	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.868		Crippen Method
mcvol	254.410	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
tb	756.82	K	Joback Method
tc	962.44	K	Joback Method
tf	420.47	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.11	J/mol×K	756.82	Joback Method
cpg	872.46	J/mol×K	928.17	Joback Method
cpg	858.26	J/mol×K	893.90	Joback Method
cpg	842.86	J/mol×K	859.63	Joback Method
cpg	826.22	J/mol×K	825.36	Joback Method
cpg	808.32	J/mol×K	791.09	Joback Method
cpg	885.50	J/mol×K	962.44	Joback Method
dvisc	0.0000636	Pa×s	756.82	Joback Method

dvisc	0.0000878	Pa×s	700.76	Joback Method
dvisc	0.0001282	Pa×s	644.70	Joback Method
dvisc	0.0002011	Pa×s	588.64	Joback Method
dvisc	0.0003470	Pa×s	532.59	Joback Method
dvisc	0.0006808	Pa×s	476.53	Joback Method
dvisc	0.0015982	Pa×s	420.47	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=U390626&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