Succinic acid, 2-methylpent-3-yl 1-cyclopentylethyl ester

Inchi: InChI=1S/C17H30O4/c1-5-15(12(2)3)21-17(19)11-10-16(18)20-13(4)14-8-6-7-9-14/h12-1

InchiKey: YEQCGBCDUREYFT-UHFFFAOYSA-N

Formula: C17H30O4

SMILES: CCC(OC(=O)CCC(=O)OC(C)C1CCCC1)C(C)C

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-346.35	kJ/mol	Joback Method
hf	-839.17	kJ/mol	Joback Method
hfus	28.73	kJ/mol	Joback Method
hvap	70.84	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.866		Crippen Method
mcvol	254.410	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
tb	754.90	K	Joback Method
tc	953.50	K	Joback Method
tf	391.57	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.73	J/mol×K	754.90	Joback Method
cpg	803.45	J/mol×K	788.00	Joback Method
cpg	821.00	J/mol×K	821.10	Joback Method
cpg	837.38	J/mol×K	854.20	Joback Method
cpg	852.63	J/mol×K	887.30	Joback Method
cpg	866.76	J/mol×K	920.40	Joback Method
cpg	879.81	J/mol×K	953.50	Joback Method
dvisc	0.0024677	Pa×s	391.57	Joback Method

dvisc	0.0009894	Pa×s	452.12	Joback Method
dvisc	0.0004923	Pa×s	512.68	Joback Method
dvisc	0.0002838	Pa×s	573.24	Joback Method
dvisc	0.0001818	Pa×s	633.79	Joback Method
dvisc	0.0001259	Pa×s	694.35	Joback Method
dvisc	0.0000925	Pa×s	754.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391410&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

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