

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	m ³ /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	Paxs	391.57	Joback Method

dvisc	0.0009894	Paxs	452.12	Joback Method
dvisc	0.0004923	Paxs	512.68	Joback Method
dvisc	0.0002838	Paxs	573.24	Joback Method
dvisc	0.0001818	Paxs	633.79	Joback Method
dvisc	0.0001259	Paxs	694.35	Joback Method
dvisc	0.0000925	Paxs	754.90	Joback Method

Sources

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=U391410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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