Succinic acid, cyclohexylmethyl cyclopentyl ester

Inchi: InChI=1S/C16H26O4/c17-15(19-12-13-6-2-1-3-7-13)10-11-16(18)20-14-8-4-5-9-14/h13-1

InchiKey: JBPAKGMTVHRLJC-UHFFFAOYSA-N

Formula: C16H26O4

SMILES: O=C(CCC(=O)OC1CCCC1)OCC1CCCCC1

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-323.00	kJ/mol	Joback Method
hf	-748.37	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	70.21	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.376		Crippen Method
mcvol	229.460	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	2145.00		NIST Webbook
rinpol	2145.00		NIST Webbook
tb	752.89	K	Joback Method
tc	970.12	K	Joback Method
tf	432.68	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.94	J/mol×K	752.89	Joback Method
cpg	805.79	J/mol×K	933.91	Joback Method
cpg	791.63	J/mol×K	897.71	Joback Method
cpg	776.09	J/mol×K	861.50	Joback Method
cpg	759.15	J/mol×K	825.30	Joback Method
cpg	740.78	J/mol×K	789.09	Joback Method
cpg	818.61	J/mol×K	970.12	Joback Method
dvisc	0.0001406	Pa×s	752.89	Joback Method

dvisc	0.0001828	Pa×s	699.52	Joback Method
dvisc	0.0002482	Pa×s	646.15	Joback Method
dvisc	0.0003560	Pa×s	592.78	Joback Method
dvisc	0.0005483	Pa×s	539.42	Joback Method
dvisc	0.0009287	Pa×s	486.05	Joback Method
dvisc	0.0017914	Pa×s	432.68	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=U391377&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