Succinic acid, hept-2-yl tetrahydrofurfuryl ester

Inchi: InChI=1S/C16H28O5/c1-3-4-5-7-13(2)21-16(18)10-9-15(17)20-12-14-8-6-11-19-14/h13-1

InchiKey: OSCZHOUXOAOTAI-UHFFFAOYSA-N

Formula: C16H28O5

SMILES: CCCCCC(C)OC(=O)CCC(=O)OCC1CCCO1

Mol. weight [g/mol]: 300.39

Physical Properties

Property code	Value	Unit	Source
gf	-436.01	kJ/mol	Joback Method
hf	-939.97	kJ/mol	Joback Method
hfus	41.16	kJ/mol	Joback Method
hvap	73.90	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.001		Crippen Method
mcvol	246.190	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	2072.00		NIST Webbook
rinpol	2072.00		NIST Webbook
tb	759.85	K	Joback Method
tc	954.50	K	Joback Method
tf	436.87	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.27	J/mol×K	759.85	Joback Method
cpg	835.90	J/mol×K	922.06	Joback Method
cpg	822.85	J/mol×K	889.62	Joback Method
cpg	808.78	J/mol×K	857.18	Joback Method
cpg	793.67	J/mol×K	824.73	Joback Method
cpg	777.51	J/mol×K	792.29	Joback Method
cpg	847.95	J/mol×K	954.50	Joback Method
dvisc	0.0001098	Pa×s	759.85	Joback Method

dvisc	0.0001443	Pa×s	706.02	Joback Method
dvisc	0.0001986	Pa×s	652.19	Joback Method
dvisc	0.0002894	Pa×s	598.36	Joback Method
dvisc	0.0004542	Pa×s	544.53	Joback Method
dvisc	0.0007871	Pa×s	490.70	Joback Method
dvisc	0.0015619	Pa×s	436.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390718&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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