Succinic acid, cyclohexylmethyl 3-heptyl ester

Inchi: InChI=1S/C18H32O4/c1-3-5-11-16(4-2)22-18(20)13-12-17(19)21-14-15-9-7-6-8-10-15/h1
InchiKey: ADMQZLXSFZZGBU-UHFFFAOYSA-N
Formula: C18H32O4
SMILES: CCCCC(CC)OC(=O)CCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-345.15	kJ/mol	Joback Method
hf	-855.41	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.402		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	782.93	K	Joback Method
tc	980.01	K	Joback Method
tf	429.32	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.45	J/mol×K	782.93	Joback Method
cpg	865.30	J/mol×K	815.78	Joback Method
cpg	882.92	J/mol×K	848.62	Joback Method
cpg	899.31	J/mol×K	881.47	Joback Method
cpg	914.51	J/mol×K	914.31	Joback Method
cpg	928.52	J/mol×K	947.16	Joback Method
cpg	941.36	J/mol×K	980.01	Joback Method
dvisc	0.0014323	Pa×s	429.32	Joback Method

dvisc	0.0006331	Pa×s	488.25	Joback Method
dvisc	0.0003336	Pa×s	547.19	Joback Method
dvisc	0.0001991	Pa×s	606.12	Joback Method
dvisc	0.0001302	Pa×s	665.06	Joback Method
dvisc	0.0000913	Pa×s	723.99	Joback Method
dvisc	0.0000675	Pa×s	782.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390603&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