

Succinic acid, cyclohexylmethyl 3-hexyl ester

Inchi: InChI=1S/C17H30O4/c1-3-8-15(4-2)21-17(19)12-11-16(18)20-13-14-9-6-5-7-10-14/h14-17
InchiKey: RBWOZNUDQLQIGM-UHFFFAOYSA-N
Formula: C17H30O4
SMILES: CCCC(CC)OC(=O)CCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-353.57	kJ/mol	Joback Method
hf	-834.77	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	71.79	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.012		Crippen Method
mvol	254.410	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	760.05	K	Joback Method
tc	957.86	K	Joback Method
tf	418.05	K	Joback Method
vc	0.963	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.48	J/molxK	760.05	Joback Method
cpg	806.22	J/molxK	793.02	Joback Method
cpg	823.76	J/molxK	825.99	Joback Method
cpg	840.11	J/molxK	858.95	Joback Method
cpg	855.29	J/molxK	891.92	Joback Method
cpg	869.31	J/molxK	924.89	Joback Method
cpg	882.19	J/molxK	957.86	Joback Method
dvisc	0.0015992	Paxs	418.05	Joback Method

dvisc	0.0007139	Paxs	475.05	Joback Method
dvisc	0.0003788	Paxs	532.05	Joback Method
dvisc	0.0002273	Paxs	589.05	Joback Method
dvisc	0.0001492	Paxs	646.05	Joback Method
dvisc	0.0001049	Paxs	703.05	Joback Method
dvisc	0.0000777	Paxs	760.05	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=U390553&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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