

Succinic acid, cyclohexylmethyl cis-hex-3-en-1-yl ester

Inchi:	InChI=1S/C17H28O4/c1-2-3-4-8-13-20-16(18)11-12-17(19)21-14-15-9-6-5-7-10-15/h3-4,
InchiKey:	YXLUKNUIEXPZFB-ARJAWSKDSA-N
Formula:	C17H28O4
SMILES:	CCC=CCCOC(=O)CCC(=O)OCC1CCCCC1
Mol. weight [g/mol]:	296.40

Physical Properties

Property code	Value	Unit	Source
gf	-270.91	kJ/mol	Joback Method
hf	-712.27	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	72.13	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.790		Crippen Method
mvol	250.110	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2183.00		NIST Webbook
rinpol	2183.00		NIST Webbook
tb	764.65	K	Joback Method
tc	965.43	K	Joback Method
tf	427.97	K	Joback Method
vc	0.949	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.73	J/molxK	764.65	Joback Method
cpg	841.56	J/molxK	931.97	Joback Method
cpg	828.01	J/molxK	898.50	Joback Method
cpg	813.37	J/molxK	865.04	Joback Method
cpg	797.63	J/molxK	831.58	Joback Method
cpg	780.76	J/molxK	798.11	Joback Method
cpg	854.06	J/molxK	965.43	Joback Method
dvisc	0.0000731	Paxs	764.65	Joback Method

dvisc	0.0000971	Paxs	708.54	Joback Method
dvisc	0.0001356	Paxs	652.42	Joback Method
dvisc	0.0002015	Paxs	596.31	Joback Method
dvisc	0.0003253	Paxs	540.20	Joback Method
dvisc	0.0005866	Paxs	484.08	Joback Method
dvisc	0.0012350	Paxs	427.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U391085&Units=SI

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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