

Sebacic acid, tetrahydrofurfuryl propyl ester

Inchi:	InChI=1S/C18H32O5/c1-2-13-22-17(19)11-7-5-3-4-6-8-12-18(20)23-15-16-10-9-14-21-16
InchiKey:	NWUGERRMNQBYOE-UHFFFAOYSA-N
Formula:	C18H32O5
SMILES:	CCCOC(=O)CCCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	328.44

Physical Properties

Property code	Value	Unit	Source
gf	-416.73	kJ/mol	Joback Method
hf	-975.97	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	78.74	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.783		Crippen Method
mcvol	274.370	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinsol	2412.00		NIST Webbook
tb	806.05	K	Joback Method
tc	998.79	K	Joback Method
tf	474.41	K	Joback Method
vc	1.054	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.85	J/molxK	806.05	Joback Method
cpg	894.34	J/molxK	838.17	Joback Method
cpg	910.70	J/molxK	870.30	Joback Method
cpg	925.97	J/molxK	902.42	Joback Method
cpg	940.16	J/molxK	934.54	Joback Method
cpg	953.29	J/molxK	966.67	Joback Method
cpg	965.39	J/molxK	998.79	Joback Method
dvisc	0.0010987	Paxs	474.41	Joback Method
dvisc	0.0005831	Paxs	529.68	Joback Method

dvisc	0.0003489	Paxs	584.96	Joback Method
dvisc	0.0002281	Paxs	640.23	Joback Method
dvisc	0.0001595	Paxs	695.50	Joback Method
dvisc	0.0001176	Paxs	750.78	Joback Method
dvisc	0.0000904	Paxs	806.05	Joback Method

Sources

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=U355718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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