

Sebacic acid, tetrahydrofurfuryl nonyl ester

Inchi:	InChI=1S/C24H44O5/c1-2-3-4-5-8-11-14-19-28-23(25)17-12-9-6-7-10-13-18-24(26)29-2
InchiKey:	SBKCDUQFWYWG NU-UHFFFAOYSA-N
Formula:	C24H44O5
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	412.60

Physical Properties

Property code	Value	Unit	Source
gf	-366.21	kJ/mol	Joback Method
hf	-1099.81	kJ/mol	Joback Method
hfus	65.40	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.123		Crippen Method
mcvol	358.910	ml/mol	McGowan Method
pc	941.52	kPa	Joback Method
rinpol	3018.00		NIST Webbook
tb	943.33	K	Joback Method
tc	1155.20	K	Joback Method
tf	542.03	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1245.58	J/molxK	943.33	Joback Method
cpg	1264.61	J/molxK	978.64	Joback Method
cpg	1282.10	J/molxK	1013.95	Joback Method
cpg	1298.11	J/molxK	1049.26	Joback Method
cpg	1312.68	J/molxK	1084.58	Joback Method
cpg	1325.85	J/molxK	1119.89	Joback Method
cpg	1337.68	J/molxK	1155.20	Joback Method
dvisc	0.0005561	Paxs	542.03	Joback Method
dvisc	0.0002767	Paxs	608.91	Joback Method

dvisc	0.0001581	Paxs	675.80	Joback Method
dvisc	0.0000999	Paxs	742.68	Joback Method
dvisc	0.0000681	Paxs	809.56	Joback Method
dvisc	0.0000492	Paxs	876.45	Joback Method
dvisc	0.0000372	Paxs	943.33	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=U355725&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
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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