

Sebacic acid, tetrahydrofurfuryl heptyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C22H40O5/c1-2-3-4-9-12-17-26-21(23)15-10-7-5-6-8-11-16-22(24)27-19-20-14

GSNMVRAKNCUOGL-UHFFFAOYSA-N

C22H40O5

CCCCCCCCOC(=O)CCCCCCCCC(=O)OCC1CCCO1

384.55

Physical Properties

Property code	Value	Unit	Source
gf	-383.05	kJ/mol	Joback Method
hf	-1058.53	kJ/mol	Joback Method
hfus	60.22	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.343		Crippen Method
mcvol	330.730	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
rinpol	2805.00		NIST Webbook
tb	897.57	K	Joback Method
tc	1099.61	K	Joback Method
tf	519.49	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.29	J/mol×K	897.57	Joback Method
cpg	1138.72	J/mol×K	931.24	Joback Method
cpg	1155.80	J/mol×K	964.92	Joback Method
cpg	1171.55	J/mol×K	998.59	Joback Method
cpg	1186.02	J/mol×K	1032.26	Joback Method
cpg	1199.25	J/mol×K	1065.94	Joback Method
cpg	1211.25	J/mol×K	1099.61	Joback Method
dvisc	0.0007076	Pa×s	519.49	Joback Method
dvisc	0.0003592	Pa×s	582.50	Joback Method

dvisc	0.0002081	Pa×s	645.52	Joback Method
dvisc	0.0001329	Pa×s	708.53	Joback Method
dvisc	0.0000913	Pa×s	771.54	Joback Method
dvisc	0.0000664	Pa×s	834.56	Joback Method
dvisc	0.0000505	Pa×s	897.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355723&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

Latest version available from:

<https://www.chemeo.com/cid/37-576-2/Sebacic-acid-tetrahydrofurfuryl-heptyl-ester.pdf>

Generated by Cheméo on 2025-12-24 01:23:04.106802871 +0000 UTC m=+6287581.636843525.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.