

Sebacic acid, tetrahydrofurfuryl undecyl ester

Inchi: InChI=1S/C26H48O5/c1-2-3-4-5-6-7-10-13-16-21-30-25(27)19-14-11-8-9-12-15-20-26(28)
InchiKey: HMSATPKJJQSGJN-UHFFFAOYSA-N
Formula: C26H48O5
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]: 440.66

Physical Properties

Property code	Value	Unit	Source
gf	-349.37	kJ/mol	Joback Method
hf	-1141.09	kJ/mol	Joback Method
hfus	70.58	kJ/mol	Joback Method
hvap	96.55	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	6.903		Crippen Method
mcvol	387.090	ml/mol	McGowan Method
pc	839.67	kPa	Joback Method
rinqol	3218.00		NIST Webbook
tb	989.09	K	Joback Method
tc	1214.99	K	Joback Method
tf	564.57	K	Joback Method
vc	1.502	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1372.64	J/molxK	989.09	Joback Method
cpg	1392.39	J/molxK	1026.74	Joback Method
cpg	1410.37	J/molxK	1064.39	Joback Method
cpg	1426.65	J/molxK	1102.04	Joback Method
cpg	1441.28	J/molxK	1139.69	Joback Method
cpg	1454.34	J/molxK	1177.34	Joback Method
cpg	1465.89	J/molxK	1214.99	Joback Method
dvisc	0.0004321	Paxs	564.57	Joback Method
dvisc	0.0002110	Paxs	635.32	Joback Method

dvisc	0.0001190	Paxs	706.08	Joback Method
dvisc	0.0000745	Paxs	776.83	Joback Method
dvisc	0.0000504	Paxs	847.58	Joback Method
dvisc	0.0000362	Paxs	918.34	Joback Method
dvisc	0.0000273	Paxs	989.09	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=U355727&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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/41-033-9/Sebacic-acid-tetrahydrofurfuryl-undecyl-ester.pdf>

Generated by Cheméo on 2024-04-27 18:18:35.466584345 +0000 UTC m=+16531164.387161660.

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