Sebacic acid, dodecyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C27H50O5/c1-2-3-4-5-6-7-8-11-14-17-22-31-26(28)20-15-12-9-10-13-16-21-27
InchiKey: KPNZWADOJDRTKF-UHFFFAOYSA-N
Formula: C27H50O5
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]: 454.68

Physical Properties

Property code	Value	Unit	Source
gf	-340.95	kJ/mol	Joback Method
hf	-1161.73	kJ/mol	Joback Method
hfus	73.17	kJ/mol	Joback Method
hvap	98.77	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	7.293		Crippen Method
mcvol	401.180	ml/mol	McGowan Method
pc	794.84	kPa	Joback Method
rinpol	3318.00		NIST Webbook
rinpol	3318.00		NIST Webbook
tb	1011.97	K	Joback Method
tc	1246.67	K	Joback Method
tf	575.84	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1436.71	J/mol×K	1011.97	Joback Method
cpg	1456.88	J/mol×K	1051.09	Joback Method
cpg	1475.14	J/mol×K	1090.20	Joback Method
cpg	1491.55	J/mol×K	1129.32	Joback Method
cpg	1506.20	J/mol×K	1168.44	Joback Method
cpg	1519.16	J/mol×K	1207.56	Joback Method
cpg	1530.51	J/mol×K	1246.67	Joback Method
dvisc	0.0003794	Pa×s	575.84	Joback Method

dvisc	0.0001837	Pa×s	648.53	Joback Method
dvisc	0.0001029	Pa×s	721.22	Joback Method
dvisc	0.0000641	Pa×s	793.90	Joback Method
dvisc	0.0000432	Pa×s	866.59	Joback Method
dvisc	0.0000310	Pa×s	939.28	Joback Method
dvisc	0.0000233	Pa×s	1011.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355728&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