Sebacic acid, tetrahydrofurfuryl hexyl ester

Inchi: InChI=1S/C21H38O5/c1-2-3-4-11-16-25-20(22)14-9-7-5-6-8-10-15-21(23)26-18-19-13-12
InchiKey: GGUGOBCEDFCGHR-UHFFFAOYSA-N
Formula: C21H38O5
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]: 370.52

Physical Properties

Property code	Value	Unit	Source
gf	-391.47	kJ/mol	Joback Method
hf	-1037.89	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	85.42	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.953		Crippen Method
mcvol	316.640	ml/mol	McGowan Method
pc	1132.91	kPa	Joback Method
rinpol	2702.00		NIST Webbook
tb	874.69	K	Joback Method
tc	1073.21	K	Joback Method
tf	508.22	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.44	J/mol×K	874.69	Joback Method
cpg	1136.78	J/mol×K	1040.12	Joback Method
cpg	1123.56	J/mol×K	1007.03	Joback Method
cpg	1109.14	J/mol×K	973.95	Joback Method
cpg	1093.51	J/mol×K	940.86	Joback Method
cpg	1076.62	J/mol×K	907.78	Joback Method
cpg	1148.84	J/mol×K	1073.21	Joback Method
dvisc	0.0000586	Pa×s	874.69	Joback Method
dvisc	0.0000769	Pa×s	813.61	Joback Method

dvisc	0.0001054	Pa×s	752.53	Joback Method
dvisc	0.0001527	Pa×s	691.46	Joback Method
dvisc	0.0002379	Pa×s	630.38	Joback Method
dvisc	0.0004074	Pa×s	569.30	Joback Method
dvisc	0.0007943	Pa×s	508.22	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=U355722&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