

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:	CCCCCOC(=O)CCCCCCCC(=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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001054	Paxs	752.53	Joback Method
dvisc	0.0001527	Paxs	691.46	Joback Method
dvisc	0.0002379	Paxs	630.38	Joback Method
dvisc	0.0004074	Paxs	569.30	Joback Method
dvisc	0.0007943	Paxs	508.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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