

Sebacic acid, decyl tetrahydrofurfuryl ester

Inchi:	InChI=1S/C25H46O5/c1-2-3-4-5-6-9-12-15-20-29-24(26)18-13-10-7-8-11-14-19-25(27)30
InchiKey:	JUCDRMZTSWSQON-UHFFFAOYSA-N
Formula:	C25H46O5
SMILES:	CCCCCCCCCOC(=O)CCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	426.63

Physical Properties

Property code	Value	Unit	Source
gf	-357.79	kJ/mol	Joback Method
hf	-1120.45	kJ/mol	Joback Method
hfus	67.99	kJ/mol	Joback Method
hvap	94.32	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.513		Crippen Method
mcvol	373.000	ml/mol	McGowan Method
pc	888.41	kPa	Joback Method
rinpol	3118.00		NIST Webbook
tb	966.21	K	Joback Method
tc	1184.53	K	Joback Method
tf	553.30	K	Joback Method
vc	1.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.91	J/molxK	966.21	Joback Method
cpg	1328.29	J/molxK	1002.60	Joback Method
cpg	1346.01	J/molxK	1038.98	Joback Method
cpg	1362.15	J/molxK	1075.37	Joback Method
cpg	1376.76	J/molxK	1111.76	Joback Method
cpg	1389.89	J/molxK	1148.14	Joback Method
cpg	1401.59	J/molxK	1184.53	Joback Method
dvisc	0.0004909	Paxs	553.30	Joback Method
dvisc	0.0002419	Paxs	622.12	Joback Method

dvisc	0.0001373	Paxs	690.94	Joback Method
dvisc	0.0000863	Paxs	759.75	Joback Method
dvisc	0.0000586	Paxs	828.57	Joback Method
dvisc	0.0000423	Paxs	897.39	Joback Method
dvisc	0.0000319	Paxs	966.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355726&Units=SI
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

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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